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Effect of Surface Treatments on the Cohesive Response of Nylon 6/silica Interfaces

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Abstract : Debonding is the one of the fundamental damage mechanisms in particle field composites. This phenomenon gains more importance in nano composites because of the extensive interfacial region present in these materials. Understanding the debonding mechanism accurately, can help in understanding and predicting the response of nano composites as the interface deteriorates. The small length scale of the phenomenon makes the experimental characterization complicated and the results of it, far from real physical behavior. In this study the damage process in nylon-6/silica interface is examined through Molecular Dynamics (MD) modeling and simulations. The silica has been modeled with three forms of surfaces – without any surface treatment, with the surface treatment of 3-aminopropyltriethoxysilane (APTES) and with Hexamethyldisilazane (HMDZ) surface treatment. The APTES surface modification used to create functional groups on the silica surface, reacts and form covalent bonds with nylon 6 chains while the HMDZ surface treatment only interacts with both particle and polymer by non-bond interaction. The MD model in this study uses a PCFF force field. The atomic model is generated in a periodic box with a layer of vacuum on top of the polymer layer. This layer of vacuum is large enough that assures us from not having any interaction between particle and substrate after debonding. Results show that each of these three models show a different traction separation behavior. However, all of them show an almost bilinear traction separation behavior. The study also reveals a strong correlation between the length of APTES surface treatment and the cohesive strength of the interface.

Keywords : debonding, surface treatment, cohesive response, separation behaviour
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