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Improving the interfacial strength of carbon fiber/vinyl ester resin composite by self-migration of acrylamide: a molecular dynamics simulation

Weiwei Jiao^a, Wenbo Liu^{a}, Fan Yang^b, Long Jiang^b, Weicheng Jiao^b, Rongguo Wang^{b**}*

^a School of Materials Science and Engineering, Harbin Institute of Technology, Harbin 150001, China.

^b Center for Composite Materials and Structures, School of Astronautics, Harbin Institute of Technology, Harbin 150080, China.

ABSTRACT. A molecular dynamics simulation was performed to investigate the migration of acrylamide (AM) to the carbon fiber (CF) surface from a liquid vinyl ester resin (VE), as well as the effect on the interfacial strength of CF/VE composite. The analysis of monomer concentration profile after the system equilibrium shows that an AM-rich interphase region was formed and the interfacial bond energy was increased. This can be explained by the greatest average atomic binding energy of AM with the CF surface. The migration of AM was confirmed experimentally by a depth profiling method using plasma etching and X-ray photoelectron spectroscopy. The AM molecules in interphase could chemically bond CF surface and VE matrix. As a result, the interface shear strength and interlaminar shear strength of CF/VE composite were enhanced by 126.98% and 81.86%, respectively.

* Corresponding Author. E-mail addresses: liuwenbohit@163.com (Wenbo Liu)

** Corresponding Author. E-mail addresses: wrg@hit.edu.cn (Rongguo Wang)

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