Silica/Epoxy interface shear debonding: interlocking or van der Waals forces? Insights from Molecular Dynamics.

Koochul Ji[a*] and Chloé Arson[b]

[a] Samsung Fire & Marine Insurance, Seocho-gu, Seoul, Korea
[b] Georgia Institute of Technology, Atlanta, GA, USA
* corresponding author: koochulji@gmail.com

Abstract: According to the early works of Sasse and Fiebrich[1], the strength of bi-material interfaces is caused by mechanical interlocking induced by the percolation of one material into the voids of the other and by van der Waals forces. In this talk, we present concrete/epoxy sliding simulations at a molecular scale to understand the relative influence of interlocking and van der Waals forces on interface shear strength. A Molecular Dynamics (MD) model of silica/polymethylmethacrylate interface is proposed, in which the silica substrate is either smooth or rough. Rough interfaces are generated by simulating Nano-imprint lithography (NIL), which is a promising technology to fabricate nanometer-scale patterns, generate rough interfaces and inject a polymer into a notched crystalline substrate like silica. After describing the construction of the MD interface model between a silica substrate with a slit-shaped cavity and High Molecular Weight Methacrylate (HMWM) with different chain lengths, we explain how to simulate the flow of polymethylmethacrylate into the silica cavity under different pressure and temperature conditions. We calculate the filling ratio of polymethyl- methacrylate, and we simulate interface sliding with and without a notch. Results show that shear strength increases with the length of the polymer chains. Interfaces with a notch have a shear strength up to 1.5 times the shear strength of an interface without a notch, which suggests that concrete reparation is more effective when the polymer is applied on rough surfaces. The work needed to propagate a fracture at the concrete/polymer interface is similar for smooth and rough surfaces. The polymer fails first even when the interface system is built with a smooth silica substrate.

[1] Sasse, H. R. and Fiebrich M. (1983). Bonding of polymer materials to concrete, Materiauxet Construction.