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Atomistic modelling of co-cured thermoplast/thermoset polymer interfaces

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Co-curing of a thermoset (TS) epoxy matrix in contact with thermoplastic (TP) foils is an essential step in a damage-free joining of polymers or polymer-based composites. However, to date, the molecular topology of the resulting hybrid TS/TP interfaces is not known. Also, it remains to be explored whether only physical (non-covalent) interactions between the two components occur, or if instead, and under which conditions, covalent bonds may form as a result of the TS resin chemically reacting with the TP chains. Such details are challenging to resolve via experimental approaches alone, which motivates the use of all-atom molecular simulation techniques in order to shed light on the details of the hybrid interface. Using polyvinylidene difluoride (PVDF) and a multicomponent epoxy resin as model systems, we have developed a computational co-curing protocol that ensures both adequate structural representation and mobility of the PVDF chains and a realistic cross-linking conversion and topology of the epoxy resin. As a result, we reveal that mutually entangled loops of thermoplastic chains and resin strands from across the interface within the extended interphase region separating the two polymers. In tensile stress simulations, we find that these loops contribute to a surprisingly large interfacial strength. In the absence of extrinsic defects, failures nucleate at the PVDF side of the interphase and propagate via a chain-pullout mechanism characteristic of semi-interpenetrating polymer networks involving thermoplastic materials. The possibility of chemical reactions between the epoxy molecules and the polar PVDF chains is explored by means of quantum mechanical calculations at the level of Density Functional Theory. Finally, the kinetics of the diffusion and co-curing conversion processes are estimated via a mesoscopic model based on the numerical solution of reaction-diffusion equations able to reproduce characteristic experimental thicknesses of the TS/TP interface region.

Biography

Lucio Colombi Ciacchi gained a PhD in materials science in 2002 and holds the Hybrid Materials Interfaces chair at the University of Bremen since 2008. He is the Speaker of the MAPEX Center for Materials and Processes and Coordinator of the interdisciplinary study program "Process-Oriented Materials Research". He has published more than 90 peer-reviewed papers in materials engineering, chemistry, and physics. His research is devoted to the atomic-scale study of interfaces between different materials and phases, with particular interest in bio-hybrid and soft-matter/hard-matter interfaces, combining both modelling and experimental techniques.

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