29 JUNE - 3 JULY
ACEX2026
RHODES · GREECE
19th International Conference on Advanced
Computational Engineering and Experimenting
29 JUNE – 3 JULY 2026 | RHODES, GREECE

ABSTRACT:

Characterization of Mechanical Interphases in Epoxy-Aluminium Joints with Coarse-Grained Molecular Dynamics

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In adhesive joints, the substrates influence the adhesive in their immediate vicinity, creating interphases with altered microstructures, which are not yet understood from an engineering perspective. A novel coarse-grained molecular dynamics (CGMD) model for adhesive joints is introduced, which allows to study the interphase formation and its properties at the molecular level. We utilize a reactive epoxy model from the literature for the adhesive and implement matching aluminium substrates, along with the necessary adherend-adhesive interaction parameters. The resulting adhesive joint model allows to investigate the formation of the adhesiveís nanostructure during curing and the mechanical properties of the joint. A parameter study on the adherend-adhesive interaction parameters unravels the role of grafting bonds and their distribution, together with the impact of the adhesiveís thickness. We identify an interphase based on variations in the local structure, estimate its size, and determine the influencing parameters. We demonstrate the capabilities of our model to evaluate the mechanical behavior of the interphase, which is crucial for gaining a better understanding of adhesive joints.