

# NANOSCALE MODELING OF COMPOSITE INTERFACE USING COMPUTATIONAL TECHNIQUES BSTRACT TITLE

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## 1. Introduction

Epoxy composites are increasingly used in various structural applications, in particular now in aerospace applications. Since large composite parts are more difficult to manufacture, sometimes it becomes necessary to join composite parts with adhesives. These adhesives must be compatible with the composite material, and ideally should have the same or better properties as the composites. The integrity of the adhesion depends on various factors, particularly the interactions associated with the chemical units in the adhesive and the composites. Although the behavior of the interface also depends on the morphology of the adhesive layer, the morphology itself depends largely on the chemical structure and interactions of the molecular units in the system. In this work, the morphological development at the interface and the corresponding properties are investigated, with particular importance to epoxy composites.

## 2. Methods

Apart from experimental techniques, which are laborious when used to investigate interface structure and properties, computational techniques are becoming more useful in understanding the structure-property relations for composite interfaces. Among other methods, molecular dynamics simulation (MD) approach was extensively used for understanding the behavior of the interface. In this work MD simulations was used to understand the morphological development of the interface when the interface is formed, as well as to estimate mechanical properties of the interface. Dependence of interface properties on the physical morphology, and hence on the chemical structure, was investigated.

There are a number of variables in this problem: structure of cross-links, nature of epoxy repeat units, density variation at the interface compared to the bulk composite, nano-scale uniformity of the interface, moisture content, etc. The dependence of morphology and properties on these parameters were investigated in detail. Presence of longer chains results in larger non-uniformities and lower strength and stiffness and results in damage at higher temperatures. Uniformity at small scale plays a significant role in defining the integrity and durability of interfaces. The degree of uniformity is characterized by a number of parameters, such as cross-link density, monomer concentration, molecular orientation aspects, etc., from the results obtained from MD simulations. Although MD simulations can be applied to short

time scales and small length scales, results from molecular level computational effort has provided significant insight into morphological aspects and mechanical properties, which were comparable to corresponding experimental values. In the cases we studied, MD results could be translated to continuum level properties with proper modifications, thus relating molecular architecture with bulk interface properties.

### 3. Conclusion

The molecular architecture, morphological structure, and interface behavior were characterized using MD simulations. The results we obtained provided insight into the conditions that must be used in the manufacturing process to optimize interface properties. In addition, aspects related to durability of the interface were also elucidated from these simulations. Computational results were compared with experimental results when possible, and good comparisons were obtained.

### REFERENCES

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