Deep Neural Networks for Predicting the Mechanical Properties of Glassy Polymer Nanocomposites

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Creating innovative materials with superior properties has been a core engineering challenge since the early days of science. Within this context, modeling and testing rationally designed polymer based nanocomposites (PNCs) is an emerging field that can yield novel materials with superior mechanical properties and added functionalities [1].

Here we propose a computational methodology for predicting the distribution of the mechanical properties in atomistic polymer-based nanostructured systems. The use of atomistic simulations is key in unravelling the fundamental mechanical behavior of composite materials. Most simulations involving the mechanical properties of PNCs concern their global (average) properties, which are typically extracted by applying macroscopic strain on the boundaries of the simulation box and calculating the total (global) stress by invoking the Virial formalism over all atoms within the simulation box; hence, extracting the pertinent mechanical properties from the corresponding stress-strain relation [2-3]. However, in order to probe the distribution of mechanical properties within heterogeneous multi-component polymer-based systems, a detailed computation of stress and strain fields for each atom within the simulation box is necessary, as shown recently by H. Reda *et al.* [4].

Starting from a recent work, we introduce a Machine Learning (ML) approach to probe the distribution of mechanical properties in heterogeneous glass polymer nanocomposites by directly computing the stress and strain at the atomic level, and averaging over all atoms within the simulation box to compute the global strain. With ML we train a U-net based network, which takes as input information about every atom in the system and predicts their corresponding stress and strain. The proposed ML tool eliminates the complexity of using complicated physical based relations, while managing to reduce the computation time by several orders of magnitude.

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