

Ultimate Uniaxial Tensile Strength of n-Alkane Glasses Determined via the Energy Landscape Formalism

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Ultimate tensile strength provides a qualitative measure of a material's overall mechanical strength and is an important property to consider in any engineering application. Experimental determination of this particular property inevitably involves destructive testing, which can be potentially expensive for materials that are difficult to produce, and it is thus desirable to predict ultimate mechanical properties using nondestructive methods. Theory and computer simulation therefore play an important role in this respect. Although crystalline materials have traditionally been the focus of research efforts devoted to the prediction of mechanical properties, glasses, or amorphous solids, have received comparatively little attention in this regard in spite of their ubiquity in modern technology. In this work, a computational methodology based on the so-called energy landscape formalism [1] is used to determine the ultimate tensile strength of glasses under uniaxial tension.

While the potential energy hypersurface, or the energy landscape, has provided a wealth of information about the vitreous state of matter at the molecular level, only recently have attempts [2] emerged to exploit this formalism computationally as a predictive tool. Here, we construct the so-called equation of state of an energy landscape to determine the ultimate uniaxial tensile strength of glasses composed of n-alkane molecules. We present results from a systematic investigation of uniaxial tensile strength in these amorphous solids as a function of chain length and system size. Interestingly, it is found that the uniaxial tensile strength varies non-monotonically with chain length but also increases with decreasing system size, where the latter trend strongly suggests that mechanical failure is governed by an intrinsic distribution of weak spots within a material.

[1] F.H. Stillinger and T. Weber, Phys. Rev. A 25, 978 (1982).

[2] V.K. Shen, P.G. Debenedetti, and F.H. Stillinger, J. Phys. Chem. B 106, 10447 (2002).