David E. Hanson holds BS and MA degrees in physics from the University of Oregon and the University of California at Santa Barbara, respectively. He is recently retired from the Los Alamos National Laboratory, Theoretical Division in the Molecular Physics and Theoretical Chemistry Group. In addition to the theory of rubber elasticity, he has contributed to a number of projects, including Molecular Dynamics simulations of reactive ion/surface interactions, Inertial Confinement Fusion and the development of micromechanical models for filled polymers. He is also a long time devotee of music and the viola da gamba early.

A New Paradigm for the Molecular Basis of Rubber Elasticity

The molecular basis for rubber elasticity is arguably the oldest and one of the most important questions in the field of polymer physics. The theoretical investigations began in earnest almost a century ago with the development of analytic thermodynamic models, based on simple, highly-symmetric configurations of so-called Gaussian chains, i.e. polymer chains that obey Markov statistics. Numerous theories have been proposed over the past 90 years based on the ansatz that the elastic force for individual network chains arises from the entropy change associated with the distribution of end-to-end distances of a free polymer chain. There are serious philosophical objections to this assumption and others, e.g., all network nodes undergo a simple affine motion and all network chains have the same length. Recently, we have proposed a new paradigm for elasticity in rubber networks that is based on physical mechanisms that originate at the molecular level. Using conventional statistical mechanics analyses, Quantum Chemistry, and Molecular Dynamics simulations, the fundamental entropic and enthalpic chain extension forces for polyisoprene (natural rubber) have been determined, along with estimates for the basic force constants. Concurrently, the complex morphology of natural rubber networks (the joint probability density distributions that relate the chain end-to-end distance to its contour length) has also been captured in a numerical model (EPnet). When molecular chain forces are merged with the network structure in this model, it is possible to study the mechanical response to tensile and compressive strains of a representative volume element of a polymer network. As strain is imposed on a network, pathways of connected taut chains, that completely span the network along strain axis, emerge. Although these chains represent only a few percent of the total, they account for nearly all of the elastic stress at high strain. We will provide a brief review of previous elasticity theories and their deficiencies, and present the new paradigm with an emphasis on experimental comparisons.

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