Physics of Liquids and Glasses

I. Understanding the structure and dynamics

Liquids and glasses are condensed-matter, in which atoms are strongly correlated in space and time. However, the correlations are short-range and dynamic, without any symmetry, making it impossible to apply theories developed for crystalline solids to describe them. For instance phonons, which are the elementary excitations of lattice dynamics in crystals, are strongly damped, and cannot be the basis for statistical mechanics in liquids and glasses. In the absence of the first-principles theories phenomenological theories, such as the energy landscape theory and mode-coupling theory, have been developed. Whereas they describe some unique features of the dynamics of liquids and glasses quite well, their microscopic foundations are unclear. We have developed a new theory, topological fluctuation theory (TFT), based upon the concept of atomic-level stresses [1], to describe the dynamics and structure of metallic liquids and glasses. The atomic-level stresses are directly related to the local topology of near neighbors of atoms. For instance the atomic-level pressure is linearly related to the number of nearest neighbors, or the coordination number. Interestingly we discovered that the self-energies of the atomic-level stresses accurately follow the equipartition theorem in high-temperature liquids, suggesting that they are the quasi-particles of atomic dynamics [2]. We use these stress fluctuations as the basis for statistical mechanics of liquids to predict their behavior, including the crossover to the energy-landscape influenced regime [3].

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II. The secrets of the glass transition

The viscosity of a liquid just above the melting temperature of a solid is of the order of centi-poise. When a liquid is supercooled without crystallization viscosity increases rapidly, until a liquid becomes a glass at the glass transition, which is defined by viscosity reaching 10^{13} poise. Why viscosity increases so rapidly over a relatively small temperature range and why a liquid becomes a glass has been a mystery for a long time. P. W. Anderson calls it one of the deepest unsolved problem in theoretical physics [1]. The topological fluctuation theory (TFT) we developed provides a convincing answer to this long-standing question. According to the TFT the square of the atomic-level stress amplitude extrapolates to zero at $T = 0$. However, the frustrations in the local atomic structure prevents such a state to be reached, and the system deviates from equilibrium, freezing into the glassy state. Freezing is spatially and temporarily inhomogeneous, with some atoms behaving like liquids while others behaving like solids. The glass transition occurs when the density of the liquid-like atoms exceeds the percolation limit [2]. The glass transition temperature thus calculated agrees with experimental results with high accuracy [2]. The theory also elucidates the structural relaxation in metallic glasses [3,4].

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Lattice Effects on the Superconductivity in Fe Pnictides

High-temperature superconductivity (HTSC) in the cuprates was discovered by Bednorz and Müller in 1986, but its microscopic origin is still unclear. Recently a group of Fe pnictide compounds were found to have the superconducting critical temperature up to 56 K, and joined the family of HTSC compounds. Both in the cuprates and pnictides strong magnetic excitations that are sensitive to superconductivity were observed [1], and a role of spins is strongly suspected. In the pnictides spin polarization occurs due to the spin-splitting of the Fe itinerant band, and is very sensitive to the lattice through the position of the pnictide ions, such as As. For this reason the As phonons couple strongly to spins. In this talk I review the properties of the FeAs superconductors, focusing on the spin excitations and spin-phonon coupling, and suggest that the spin-phonon coupling must be intimately involved in the superconductivity of this family of compounds.

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