Rigidity as a tool to understand the role of low frequency modes in glass transition and flexible systems

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Very recently, rigidity theory has been used as a tool to understand in a unified way physical trends in many diverse systems, like in glasses, polymers, fluids, colloids, granular material, proteins and even in computational complexity. The basic idea behind this approach is to treat bonding as a mechanical constraint. In this talk, we will show that such universality stems form the fact that rigidity theory provides a useful description of the energy landscape of flexible systems [1], and thus many thermodynamical and relaxational properties are related to it.

As an example, we discuss the case of glass transition. Although there are many theories to understand this transition, most of them just ignore a fundamental fact: all glasses have an excess of low-frequency vibrational modes. Here, the effects of flexibility and chemical composition in the variation of the glass transition temperature are obtained by using the Lindemann criteria, that relates melting temperature with atomic vibrations. Using this criteria and that low frequencies vibrations enhance in a considerable way the average quadratic displacement, we show that the consequence is a modified glass transition temperature [2]. This approach allows to obtain in a simple way the empirically modified Gibbs-DiMarzio law, which has been used in chalcogenide glasses to fit the changes in the glass transition temperature with the chemical composition. Other known relationships are also obtained, like the Tanaka law and the 2/3 law relating melting and glass transition temperatures.

Finally, we discuss the effects of flexibility in the relaxation properties. This is done by making the observation that relaxation takes place mainly due to non-linear interactions, with an energy cascade mechanism that transfers energy from high to low frequency modes, where energy is dissipated due to their quasiresonant nature. Since flexibility enhances the number of low-frequency modes, the relaxation properties are changed and stretched exponentials are observed with an exponent that depends upon the rigidity of ths system.

[1] G.G. Naumis,Phys. Rev. E71, 026114 (2005).

[2] G.G. Naumis, Phys. Rev. B 73 (Brief Report), 172202 (2006).