

Abstract Submitted
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The role of low frequency vibrational modes localization properties in the glass transition and mechanical stability of glasses GERARDO NAUMIS, Depto. de Física-Química, Instituto de Física, UNAM — It is surprising that although glasses present low frequency vibrational anomalies like floppy modes or the Boson peak, not so much effort has been made in order to understand the relationship between glass transition and low frequency anomalies, which we know are fundamental in the stability of solids. We will show that rigidity theory allows to understand in a systematic way such relationship. Then, 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, and rigidity theory. Using this criteria and that floppy modes at low frequencies enhance in a considerable way the average quadratic displacement, we show that the consequence is a modified glass transition temperature. This approach allows to obtain in a simple way the empirically modified Gibbs-DiMarzio law, which has been widely used in chalcogenide glasses to fit the changes in the glass transition temperature with the chemical composition [1]. The method predicts that the constant that appears in the law depends upon the ratio of two characteristic frequencies (or temperatures). This constant is estimated for the $\text{Se}_{1-x-y}(\text{Ge}_y\text{As}_{1-y})_x$ glass by using the experimental density of vibrational states, and the result shows a good agreement with the experimental fit from glass transition temperature variation. [1] G.G. Naumis, Phys. Rev. B 73, 172202 (2006).

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