

# **Fragility, activation volume, and correlation volume: A triple of essential parameters that characterize molecular dynamics of glass formers under high pressure**

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## **Abstract:**

The fragility parameter is considered to provide a meaningful characteristic of molecular dynamics of glass forming liquids, because it successfully describes the sensitivity of the molecular dynamics of materials approaching the glass transition to changes in temperature. However, the high pressure study of the glass transition and related phenomena shows [1] that also other parameters can play an important role in the understanding of the dramatic slowdown in molecular dynamics near the glass transition. In this context, we intend to present results of our latest studies devoted to the activation volume [2] and the dynamic heterogeneity [3] in relation to the fragility parameter of glass formers under high pressure. Although the fragility parameter is discussed as a function of pressure, the activation volume is the basic parameter that characterizes the sensitivity of the molecular dynamics near the glass transition to changes in pressure. Our recently derived equations of state for volume [4] and activation volume [2] as well as the pressure coefficient of the glass transition temperature  $dT_g/dp$  [5], which are well interpreted in the density scaling regime, give a new insight into the interrelation between the important parameters such as isobaric fragility, activation volume and  $dT_g/dp$ . Consequently, we show how the fragility parameter can be expressed by using volumetric data. Finally, we discuss [3] the dynamic heterogeneity of molecular dynamics under high pressure within the formalism of the four point correlation function. We verify whether any correlation exists between the correlation volume defined by the height of the peak of the four point dynamic susceptibility function and the fragility and activation volume parameters investigated in high pressure conditions.

## **References:**

- [1] G. Floudas, M. Paluch, A. Grzybowski, and K. Ngai, *Molecular Dynamics of Glass-Forming Systems: Effects of Pressure*, Chap. 1, Springer-Verlag Berlin Heidelberg 2011.
- [2] A. Grzybowski, K. Koperwas, A. Swiety-Pospiech, K. Grzybowska, M. Paluch, *Phys. Rev. B* 87, 054105 (2013).
- [3] A. Grzybowski, K. Kolodziejczyk, K. Koperwas, K. Grzybowska, M. Paluch, *Phys. Rev. B* 85 (2012) 220201(R); arXiv:1302.5136v2.
- [4] A. Grzybowski, K. Grzybowska, M. Paluch, A. Swiety, K. Koperwas, *Phys. Rev. E* 83, 041505 (2011).
- [5] K. Koperwas, A. Grzybowski, K. Grzybowska, Z. Wojnarowska, J. Pionteck, A. P. Sokolov, and M. Paluch, *Phys. Rev. E* 86, 041502 (2012).