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Geometry and Physics of Covalent Network Glasses

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Glasses are characterized by the absence of long-range order which defines crystalline materials. However, they possess a rich and varied array of short to medium range order, which originates from chemical bonding and related interactions. whereas covalent systems (mostly chalcogenides like As-Se, Ge-AsSe systems) or oxides (borate, boro-silicate and silicate glasses), have sparsely packed, strongly bound network structures, like tetrahedral SiO2 units or B3O3 boroxol rings. These very different structures results in different physical properties and applications.
We present a simple mathematical model of glass transition based on the analysis of molecular agglomeration in overcooled liquids. The model uses the space of probabilities of appearance of given local structures, and their slow time evolution during annealing from a liquid melt. The evolution of probabilities is described as action of an appropriate stochactis matrix. The glass transition is defined as a fixed point resulting from the requirement of maximal homogeneity. With simple assumptions concerning local configurations and their bonding energies, and with elementary combinatorics we are able to derive the dependence of the glass transition temperature Tg on chemical composition in non-organic covalent glasses. Numerous examples are shown to confirm the validity of the stochastic agglomeration model.

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