A dynamic facilitation approach to the melting kinetics of stable glasses

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The dynamic facilitation perspective underlying the study of kinetically constrained models (KCMs) aims to shed light on the physics of the glass transition without resorting to any unobserved non-trivial thermodynamics [1]. In these models, the stochastic dynamics is given in terms of mesoscopic variables that reflect the local density of an underlying glass former, and are subject to *kinetic constraints*, i.e. local update rules that give rise to glassy relaxation patterns.

Our aim is to elucidate the dynamics of stable glasses by studying KCMs. By stable glasses we refer to glasses prepared by physical vapour deposition (i.e. by depositing molecules from a gas gradually onto a low temperature substrate) at a deposition temperature $T_{\rm dep}$ that is slightly below the experimental glass transition temperature T_g [2]. These systems have been experimentally shown to possess very high thermodynamic and mechanical stabilities as compared to ordinary glasses prepared by bulk cooling, an intringuing feature for which a satisfying explanation is still lacking.

In a recent work, we aim to reproduce the kinetics of melting, i.e. the evolution towards equilibrium when the temperature is suddenly increased above T_g, in stable glasses [3]. The melting phenomenology presents one of the most striking differences between stable and ordinary glasses: while ordinary glasses melt in a homogeneous fashion, stable glass melting is characterised by the appearance of a front that propagates ballistically from the deposition surface [4].

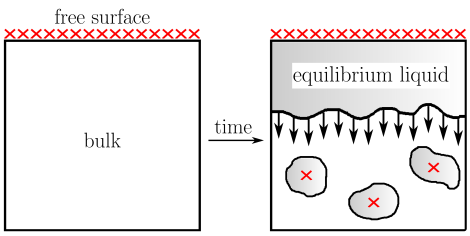

Figure 1: **Stable glass melting**. Initially, there is a top layer of excitations and an empty bulk. As time proceeds, a front propagates from the top layer and new isolated excitations are sponatenously created (nucleate) and grow in the bulk.

To this end, we use a soft KCM (i.e. a model where excitations – i.e. liquid-like regions – can appear spontaneously), which is a 3D generalisation of the soft East model [5]. Such system is studied in a configuration that mimics the experimental conditions of stable glasses after preparation. Initially, there are excitations only on the highly mobile free surface, but as time proceeds, a front propagates into the system, see Fig. 1. The soft constraint allows for excitations to appear in the bulk, which may occur before the front has fully transformed the system or not depending on the thickness of the sample, as has been observed [4]. Bulk relaxation and front propagation compete in the melting dynamics.

This simple model reproduces the phenomenology of stable glass melting [4]. Furthermore, it allows us to probe front and bulk separately, thus providing insight into the origin of the crossover that results from the above mentioned competition, as illustrated in Fig. 2, where $1-p(t)$ is effectively the fraction of the liquid ($p(t)$ is the persistence). In agreement with recent experimental and theoretical work, we find the bulk relaxation to follow an Avrami equation [6], $1-p(t) = 1-\exp(-k\,t^n)$ and provide insight into the anomalous exponents that are observed. A generalisation of this equation that encompasses both front and bulk relaxation (see F+B in Fig. 2) has been recently found [8].

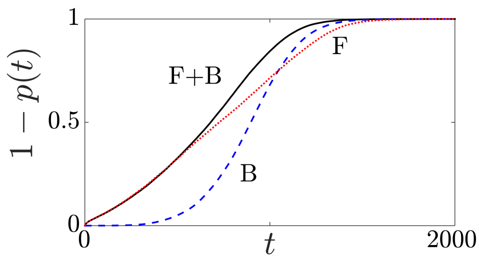

Figure 2: **Front and bulk relaxation**. Transformation of a $64\times64\times64$ lattice at $T=0.45$ as given by the fraction of spins that have flipped at least once $1-p(t)$: (F) front propagation, (B) bulk relaxation, (F+B) both combined.

Current efforts aim to generalise the model so as to include a *fictive temperature field* that couples the energy barrier for spontaneous excitation to the dynamics [8]. This will bring us closer to experimental reality, yielding a propagation speed that depends on the stability [7], thus allowing us to shed light on the length characterising the crossover between front-dominated and bulk-dominated relaxation. With the new model we can moreover *produce* stable glasses [9], as well as ordinary glasses, and study the history-dependent properties resulting from their preparation.

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