



Charge density glass dynamics – Soft potentials and soft modes

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ABSTRACT

An universal fingerprint of glasses has been found in low-temperature thermodynamic properties of charge/spin density wave (C/SDW) systems. Deviations from the well-known Debye, elastic continuum prediction for specific heat (flat C_p/T^3 plot) appear as two anomalies; the upturn below 1 K and a broad bump at $T \sim 10$ K (named Boson peak in glasses). The first one, inherent of localized two level systems within the shallow corrugated phase space, exhibits slow relaxation with the complex dynamics. The second one, “Boson peak-like peak” was attributed to the pinned mode and incomplete softening of CDW *superstructural* mode. We discuss similar $C_p(T)$ features found also in incommensurate dielectrics with well documented soft-mode anomalies.

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The only story that never changes, one that does not come and does not go and is in the background of all stories, is the story about waves and the sea.... How can a wave, no matter how brave, proclaim itself to be just a wave, forgetting that it is the sea?

..... The highest peak of the wave-man is his recognition of his own oceanic nature. (Vesna Krmpotić)

1. Introduction

Ultra-low temperature (T) anomalies in specific heat C_p caused by CDW were predicted in 1978 by Boriack and Overhauser [1].

They have calculated the phase excitation contribution and illustrated the characteristic signatures of phasons with gap-less dispersion, particularly with the aim to detect them in potassium. Eight years later we have investigated CDW system $(\text{TaSe}_4)_2\text{I}$ exhibiting shallow, spoon-like anomaly instead of a pronounced Kohn anomaly (as found first in $\text{K}_2\text{Pt}(\text{CN})_4\text{Br}_{0.3} \times 3.2 \text{H}_2\text{O}$ (KCP) and later on in $\text{K}_{0.3}\text{MoO}_3$ (blue bronze) with a very characteristic calorimetric signature, which we have interpreted within a modified Overhauser's model with gaped dispersion [2]. In addition, other CDW systems investigated afterwards showed similar signatures; quasilinear contribution ($C_p \sim T^\alpha$, $\alpha \sim 1$) below 1 K and maximum in C_p/T^3 at slightly higher temperature. These are well known low- T universal features of glasses, however still not satisfactory understood. Together with other indicative properties for glassiness, as very complex slow dynamics, hysteretic behavior, memory effects, these calorimetric fingerprints of glass were strongly motivating driving force in searching the real glass transition in CDW systems, as described “...from fiction to facts” in our contribution at ECRYS 2008 [3]. We have introduced the new generic feature of DW phase diagram (including SDW systems [4,5]) which is a glass transition at $T_g \sim T_p/5$ (T_p is the DW

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transition temperature) and ultimately proven freezing criterion into the DW glass (DWG) [3,5].

In this paper we shortly review on the thermodynamic evidences of the complex dynamics of DWG within the corrugated phase space caused by specific and known DW microscopy (screening and pinning) unlike very abstract and highly generalized picture in conventional glasses. We present microscopic interpretations of Two Level States/Systems (TLS) and Boson peak (BP) inherent of DW phenomenology. We also discuss the apparent similarities with ordinary (“short range”) glasses as well as specific differences found in DWG complex dynamics due to the fact that the relevant degrees of freedom are related to the phase excitations (phasons) and not to the ill-defined phonons in glasses.

Incommensurate structures are characterized in general by a gapless (acoustic-like) phason branch, so that in searching for the ideal Overhauser’s model system, we discuss at the end also the overall similar $C_p(T)$ behavior of some IC dielectrics.

2. Universal DWG features in low- T heat capacity

We show in Fig. 1. normalized heat capacity C_p/T^3 of CDW systems o-TaS_3 , $\text{K}_{0.3}\text{MoO}_3$ and KCP. It is characterized by the upturn at lowest temperatures¹ and the maximum in C_p/T^3 in excess to the regular Debye-like heat capacity (given by flat, broken lines). These features correspond very well for $T < 1$ K to the power law contribution from low energy excitations named TLS and to the Boson peak in glasses at $T \sim 10$ K [6], as demonstrated for vitreous silica in upper panel (full line).

In the field of glasses it is argued that TLS are responsible for the low- T properties, specific heat $C_V \sim T$, thermal conductivity $\kappa \sim T^2$, sound attenuation and energy relaxations (Refs. 5 and 6 in [6]). The microscopic nature of TLS is still a mystery, but colloquially it is described as an atom/group of atoms sitting equally well in one of two positions in an asymmetric double well potential, as shown schematically in Fig. 2. in the next paragraph. It is believed that the same excitations cause BP and the plateau in $\kappa(T)$ at the same temperature. Moreover, recently a subtle connection of both phenomena with TLS manifested at a much lower temperature was indicated [6]. Especially interesting is the conclusion that the characteristics of the plateau in $\kappa(T)$ arise from calculable interactions of those degrees of freedom with the phonons [6].

As there is a very strong dependence $C_p(t_d)$ on the duration of the heat pulse t_d in DW systems [4] caused by very long relaxation time of TLS after perturbation, it indicates decoupling of TLS from the underlying phonons, the fact which can explain why $\kappa(T)$ in DW systems has regular crystalline behavior [7]. Again, this is consistent with our presumption that DWG is “superstructural” glass with ill-defined phasons, in parallel with ill-defined phonons in structural glasses responsible for heat transport.

One more distinguishing point is high sensitivity of DWG TLS to magnetic field, equally in dynamics [8,9] and thermodynamics [9,10]. $C_p(H)$ shows a peak at $\mu_B H \sim T$ for $T < 1$ K what was explained by specific soliton-like defects ([9] and references therein) and alternatively in the impurity-stabilized Luttinger liquid approach [10].

3. Corrugated phase space, soft potentials and slow dynamics

The phase excitations which govern the DW low energy properties are strongly affected by the interaction with random

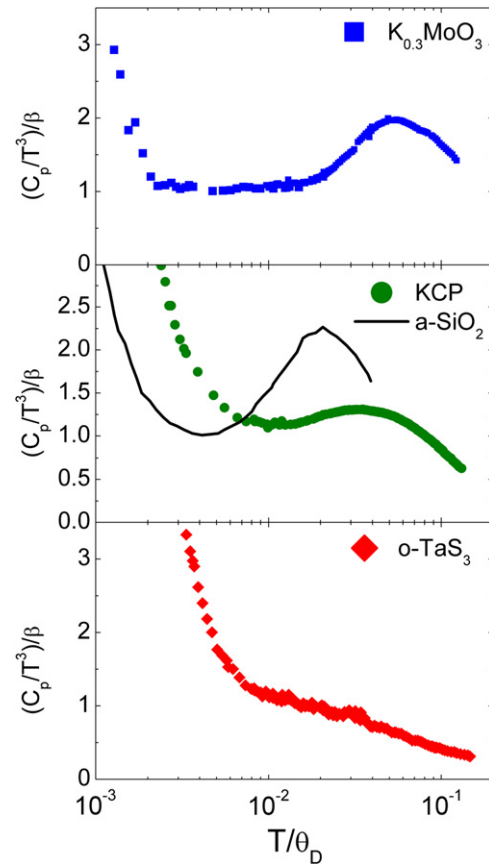


Fig. 1. Additional contributions compared to the Debye acoustic contribution βT^3 in C_p/T^3 plot vs. normalized temperature T/θ_D for CDW systems – $\text{K}_{0.3}\text{MoO}_3$, KCP and o-TaS_3 taken from ref. 13 and refs. therein. θ_D is Debye temperature for each compound, 226 K, 225 K and 202 K, respectively. Vitreous silica data are given for comparison.

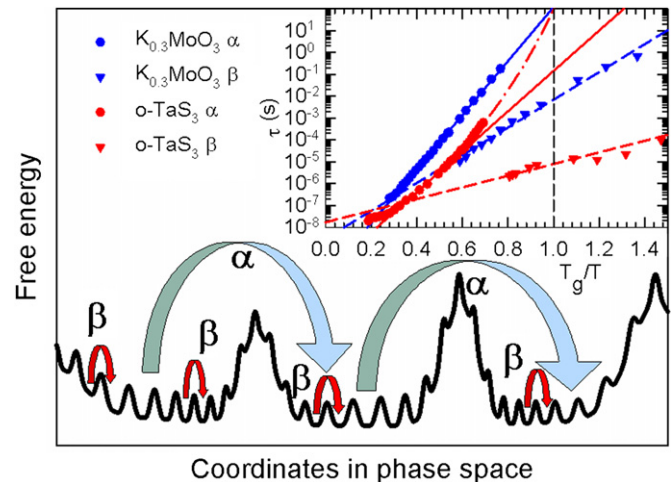


Fig. 2. Schematic presentation of the corrugated energy landscape giving rise to the complex glassy dynamics; primary, α process at $T > T_g$ is relaxation between big minima which freezes out at T_g when the barrier becomes larger than T , as demonstrated in the Arrhenius plot of the corresponding relaxation times for o-TaS_3 and blue bronze in the inset. Secondary, β process is relaxation between neighboring shallow minima, each couple as one TLS.

impurities. Impurity pinning breaks DW in the domains of correlated phase. Because of the random nature of the pinning, there are many nearly degenerate, metastable minima with energy barriers scaling with the threshold field for DW depinning. Low frequency DW dynamics in high- T weak pinning-regime

¹ Intentionally all contributions are not listed here for clarity. There is also a hyperfine-like $C_p \sim T^2$ contribution from TLS [8].

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