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Numerical simulation study of the charge density wave dynamic properties in the one-dimensional systems

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A B S T R A C T

In this work, we present a numerical simulation study of the dynamic properties of the charge density waves (CDW) in one-dimensional system. We present firstly, the results obtained within the classical model where the CDW is assimilated to a rigid particle. While this model explains qualitatively the CDW conductivity field dependence, a smooth discordance with the experimental results is observed. We present also the results obtained in the context of the deformable model where the CDW is considered as a continuum medium in interaction with the randomly distributed impurities in the lattice. The results obtained within this mode are in good concordance with the experimental ones which showing that the internal degrees of freedom play a capital role in the CDW dynamic properties.

1. Introduction

The quasi one or two-dimensional conductors have been the subject of extensive experimental and theoretical work during the past decades. These compounds undergo a structural instability of a particular type: a Periodic Lattice Distortion (PLD) with wave vector: $\mathbf{Q} = 2\mathbf{K}_F$($\boldsymbol{K}_F$ is the Fermi vector); accompanied by a modulation of the electron density called a Charge Density Wave (CDW). This instability occurs by an opens up an energy gap at the Fermi level. The PLD coupled to CDW is a direct consequence of a strong electron–phonon coupling and of a particular topology on the Fermi surface (Perfect Nesting in the quasi-one dimensional case) [1–3]. The resulting metal–insulator transition is called "Peierls transition".

Fröhlich (1954) has proposed that an incommensurate charge density wave can slide freely at no cost in energy. This collective transport of electrical current by a moving CDW would lead to superconductivity, the so-called "Fröhlich superconductivity" [4]. In real systems, the Fröhlich superconductivity is not observed, because the CDW is pinned by impurities, or lattice defects, or by eventual commensurability effects.

The interaction of impurities or defects with CDW is responsible for the existence of threshold electric field E_T, below which the CDW is pinned to randomly distributed impurities, or lattice defects. Above E_T, the nonlinear electrical conduction Properties (collective transport) observed in some quasi-one dimensional compounds such as $NbSe_3$ (1967) are attributed to the sliding motion of the CDW [5]. In addition to $NbSe_3$, several quasi-one-dimensional conductors at CDW have been shown [3,6,7]. The dynamics of the CDW systems is affected by several factors [8,9] such as: the temperature, the type of defects, the nature of impurities, and the type of the sample.

The signature of the collective excitations of the CDW ground state in the optical proprieties of one-dimensional conductors has been subject to intensive studies for many years [3]. Due to pinning of the CDW condensate by impurities or lattice defects a phase mode and an amplitude mode are expected [3a]. Within this framework Gorshunov et al. [3b] have studied the optical response of the sliding CDW in $K_{0.3}MoO_3$, they have shown the existence of two optical modes in the millimeter wave and far-infrared range which have been assigned to the amplitude and the phason mode. These results were ascribed to the sliding CDW condensate which interacts with lattice defects.

In order to understand the phenomena associated to CDW and to interpret the experimental results obtained, several models has been proposed [10–13], but neither of them can accounts all these results.

In parallel, with theoretical and experimental work, the dynamics of CDW has been studied by numerical simulations. Based on the rigid wave model [10], Servin and Salva [14] have shown that a similar phenomenon to the interference of the CDW with ac excitation in a sample of CDW polytype subjected to a dc electric field. In recent work, we have shown [15,16] the existence of a intermidiate pinning case between the strong and the weak pinning ones, as well as the existence of a effective threshold field depending on the friction coefficient and the CDW pinning phenomenon is a dynamical critical phenomenon. Using the deformable wave model, many nonlinear transport properties attributed to motion of CDW have been reproducing by several authors [17–23].

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In this letter, we study by numerical simulation the CDW dynamics properties in these two models, the deformable wave, and rigid wave model.

2. Models and results for numerical simulations

2.1. Rigid wave model

The classical model of rigid wave proposed by Grüner et al. [10], where the CDW is assimilated of a charged particle moving in a sinusoidal potential to a period λ tilted by the applied electric field. This potential is the pinning potential of the CDW by the impurities. It is noted that displacing the CDW by one period results in the same energy configuration.

For small applied electric fields, the inertia term can be neglected, when the equation of motion becomes:

$$\frac{1}{\tau}\frac{dx}{dt} + V_0 \sin(Qx) = \frac{e}{m^*}E \tag{1}$$

where 1/ is the damping coefficient, m^* is the effective mass of the CDW, V_0 is the characteristic frequency of pinning, and $\lambda = 2\pi\, Q$.

The nonlinearity of the problem comes from CDW-impurities interaction and makes it difficult to handle by an analytical method. Therefore, we have resolved numerically the Eq. (1), using the Runge–Kutta method of order 4 described by Press et al. [24].

In the incommensurate case, the pinning phenomenon results from the CDW interaction with the impurities or the lattice defects. The ground state of CDW results from the competition between the pinning force and electrical force applied from outside. Application of electric field sufficient to overcome pinning energy before the CDW begins to slide, resulting in a current-carrying.

In Fig. 1 is reported the CDW current density variation on applied electric field. This result allows to determine the threshold field E_T.

Above the threshold field E_T, the field-dependent current density follows a power law, given by:

$$J_{\mathrm{CDW}} = J_0\left[\frac{E}{E_T} - 1\right]^{\eta} \tag{2}$$

where η is an exponent damping coefficient dependent, for example: $\eta = 0.909$ for $\gamma = 0.159{\cdot}10^{-17}$ Nscm^{-1}.

This result is in agreement with experimental work obtained on samples of molybdenum blue bronzes [8,26].

The collective transport phenomenon of CDW provides an additional contribution to the conductivity resulting in a non-linear current [26–28]. In Fig. 2 is reported the field conductivity

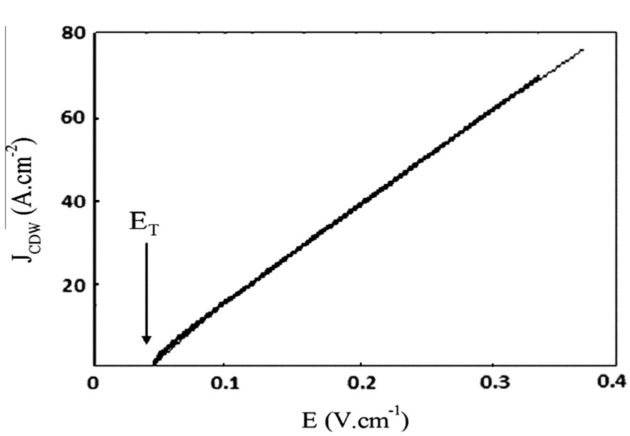

Fig. 1. Electrical field dependence of the CDW current density J_{CDW}; solid line is fit to Eq. (2).

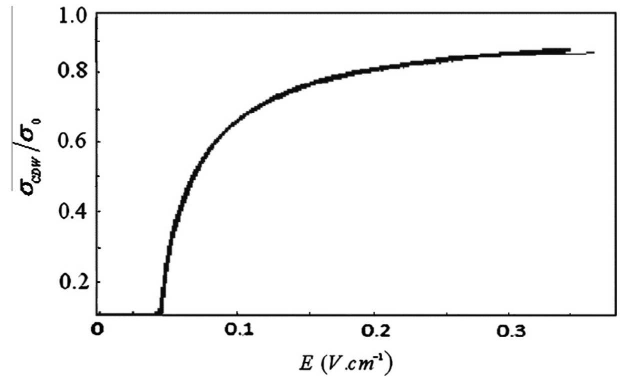

Fig. 2. Normalized CDW conductivity versus electric field; solid line is fit to Eq. (3).

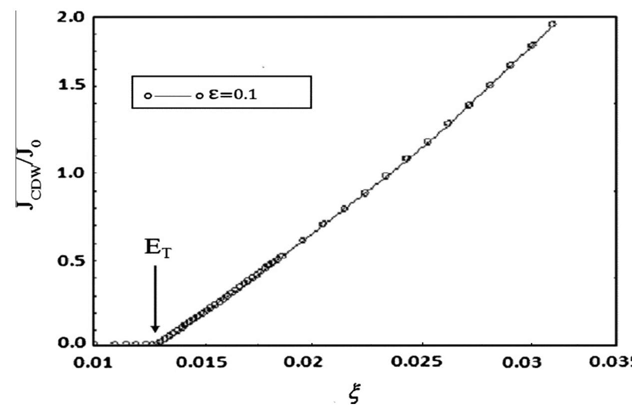

Fig. 3. Electrical field dependence of CDW normalized current density (c_i = 200 ppm); solid line is fit to Eq. (2).

dependence, showing that the CDW field conductivity dependence follows a power law, given by:

$$\sigma_{\mathrm{CDW}}(E) = \sigma_0\left[\frac{E_T}{E}\right]\left[\frac{E}{E_T} - 1\right]^{\eta} \tag{3}$$

where η is an exponent damping coefficient dependent, for example: $\eta = 0.909$ for $\gamma = 0.159{\cdot}10^{-17}$ Nscm^{-1}.

Below the threshold field E_T, the electrical conductivity σ_{CDW} is zero and increase with increasing field and it seems to reach a limiting value for high field which indicates that the conductivity is saturated for high fields. The curve in solid line represents the law of variation of electrical conductivity experimentally obtained [8,25,26]. In this model, the value of the exponent η obtained is smooth discordance with the experimental results observed (see Fig. 3).

The classical model explains qualitatively the CDW conductivity field dependence, it does not describe satisfactorily the variation of current density carried by CDW; because the experimental results [8,25,26] show that the exponent η of the law (Eq. (2)) must be greater than 1.

2.2. Deformable wave model

In the Fukuyama-Lee-Rice (FLR) [13] model, the CDW is considered as a continuum deformable medium interacting with the randomly distributed impurities in the rigid lattice. The effects of thermal fluctuations and the free electrons are neglected. Only the CDW phase fluctuations are considered, the amplitude ones are neglected. The ground state of CDW results from the