Inverse Problem for Thermal Diffusivity in $YBa_2Cu_3O_{7-x}$ Superconductor

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Abstract. Further development of of the thermal explosion model (TEM) describing track formation processes in high-T_c superconductors is suggested. Information on the temperature dependence of electron thermal diffusivity in $YBa_2Cu_3O_{7-x}$ is obtained by solving an inverse problem of reproducing measured track radii.

Nanodimension ion track technologies are now of great importance, in particular for their enabling increase the critical current density in high-T_c superconductors. In spite of the manifest practical significance, until now there is no satisfactory theory of track formation for these materials. Although different mechanisms were suggested till now, thermal spike (TSM) and thermal explosion (TEM) models were demonstrated to be most matchable for this purpose (see [1, 2, 3] and references therein). Mathematical modeling of track formation in $YBa_2Cu_3O_{7-x}$ using TSM revealed some unexpected peculiarities of the process such as impossibility to formulate an appropriate Stephan problem, existence of the electronic quenching phenomenon resulting in supersensitivity of track radii to small variations of electron diffusivity value [2], which requires a logical design of special computing circuits. It was shown in [3] that taking into account superheating nonequilibrium processes allows one to stabilize the model and obtain a quantitative description of tracks in $YBa_2Cu_3O_{7-x}$ with both elliptical and circular cross sections.

In the present paper, another even more crucial problem is considered. The fact is that electron thermal diffusivity, D_e, was considered previously as an adjustable parameter of thermal spike and thermal explosion models for varying types and energies of impinging ions. Meanwhile, the self-consistency of the theory requires to use a single function, depending on electron temperature in the superconductor, $D_e(T_e)$, for the whole bulk of data. We show here that such a function really exists and takes quite reasonable physical values [4].

TSM assumes the following system of two coupled nonlinear differential equations for electron, T_e, and atom, T_i, temperatures:

$$\rho C_e(T_e)\frac{\partial T_e}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rK_e(T_e)\frac{\partial T_e}{\partial r}\right] + \qquad (1)$$

$$\frac{1}{r^2}\frac{\partial}{\partial \varphi}\left[K_e(T_e)\frac{\partial T_e}{\partial \varphi}\right] - g\cdot(T_e - T_i) + q(r,\varphi,t),$$

$$\rho C_i(T_i)\frac{\partial T_i}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rK_i(T_i)\frac{\partial T_i}{\partial r}\right] + \qquad (2)$$

$$\frac{1}{r^2}\frac{\partial}{\partial \varphi}\left[K_i(T_i)\frac{\partial T_i}{\partial \varphi}\right] + g\cdot(T_e - T_i).$$

Initial conditions are chosen as

$$T_e(r,0) = T_i(r,0) = T_0,$$

and boundary conditions are

$$(\partial T_e/\partial r)_{r=r_{min}} = (\partial T_i/\partial r)_{r=r_{min}} = 0,$$

$$T_e(r_{max},t) = T_i(r_{max},t) = T_0,$$

where T_0 is temperature of the environment and no-heat-transfer condition at the center of track $r = r_{min}$ is taken into account. Parameter $r_{min} = 0.1$ nm is introduced to avoid difficulties with description of energy deposition at point $r = 0$, and $r_{max} = 10^{-5}$ cm is a physical infinity as used here.

If the direction of an incident ion is parallel to c axis, one can ignore the φ-dependence, and the system (1) – (2) is reduced to that used in [2] for description of tracks with circular cross sections. If the incident ion is parallel to [100] or [010] directions, the elliptical defects appear [5]. This fact was explained by an anisotropy of the thermal conductivity of $YBa_2Cu_3O_{7-x}$ in the *a*-*c* and *b*-*c* planes [3]. Corresponding calculations were fulfilled in the frame of TEM which is more stable than TSM at small variations of electron thermal diffusivity parameter, D_e.

There are the following reasons for generalization of TSM to TEM. According to TSM, almost total primary energy losses of the incident ion are concentrated in the electron subsystem, and further electron-atom energy transfer is accompanied by electron and atom heat conduction, eqs.(1)–(2). In $YBa_2Cu_3O_{7-x}$, the initial electron hot spot has time to spread over a considerable part of the track cross-section without essential heating of atoms already at the early stage of the electron-atom relaxation process, because electron thermal conductivity, $K_e \sim T_e$, is relatively large at that time. This results in almost synchronous *volumetric* electron-atom energy transfer and, consequently, in a specific melting process. Indeed, according to generally accepted views, the usual melting at equilibrium point can be described as loss of structural order in a *thin layer* near interphase boundary which gradually expands from the track center outside. This is formally in line with the Stefan formulation of the melting problem. Meanwhile, for volumetric melting, breaking the structural order takes place in an essential part of the track volume *simultaneously*. The corresponding generalized Stefan problem together with appropriate its numerical implementation is described in [6]. Definite traits of superheating can be revealed experimentally in laser-induced melting in thin films [7]. For example, ion temperature, T_i, can rise several times higher than melting temperature at the equilibrium phase transition, because of a time interval to break the atomic structure should be shorter in this case. On the base of superheating physical picture, the TEM was suggested in [3]. Thus, it uses different description of melting process, although the same system of equation, (1) and (2). A single free parameter of TEM is the temperature of superheating, T_{sh}, which describes a minimum value of atom temperature should be mounted for destroying a structural order of the substance. It was found to be nearly 4 times larger than melting temperature in $YBa_2Cu_3O_{7-x}$, $T_{sh} \simeq 5372$ K [3].

The properties of electron and atomic subsystems showing themselves in thermal physics constants in equations (1)–(2) were chosen using current experimental and theoretical knowledge on $YBa_2Cu_3O_{7-x}$ (see ref. in [1, 2, 3]). The only unknown value the thermal diffusivity in $YBa_2Cu_3O_{7-x}$ as function of electron temperature was found by the minimization of deviation of the theoretical track radii from experimental ones, in Fig. 1. It satisfies the requirement to be $\simeq 1$ cm^2/s at high temperatures, as it was predicted in [8, 9], and demonstrates a monotonous growth at $T_e > 10^4$ K, in qualitative agreement with [10]. A decrease of function $D_e(T_e)$ from $D_e \simeq 0.26 \div 0.52$ at $T_e = 300$ K to $D_e \simeq 0.01$ K at $T_e = 10^4$ K is slightly unexpected, though quite possible, and is a non trivial prediction of this variant of TEM [1].

In the TEM framework, melting is considered to be at $T_{sh} > T^*$. It is appropriate to assume a condition

$$(T_{sh} - T^*)C_i > L \tag{3}$$

implying a reasonable physical suggestion that energy spent on the non-equilibrium melting should oversize the value of L. As a result, the minimal superheating, $T_{sh} = 4T^*$, is supposed, which corresponds to the fulfillment of the condition (3) near its threshold.

[1] It turned out to be impossible to indicate an exact region where the value of $D_e(T_e)$ in Fig. 1 decreases essentially, as far as electron temperature in a large region around track, at the moment of track boundary formation, is much higher than T_0. Therefore, the region of an essential decrease, $T \simeq T_0$, shown in Fig. 1 should be considered as a rough estimation.

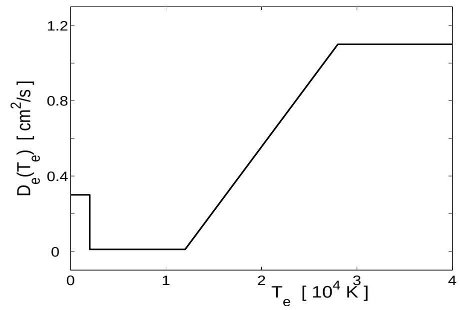

Figure 1: Thermal diffusivity in $YBa_2Cu_3O_{7-x}$ as function of electron temperature, T_e, found from the requirement imposed on TEM to account for experimental track radii

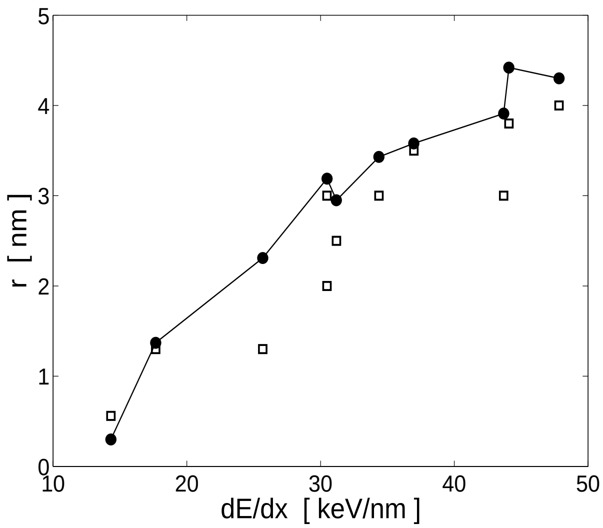

Figure 2: Experimental (squares) and theoretical (circles) track radii obtained in the TEM framework for different ions bombarding $YBa_2Cu_3O_{7-x}$.

The TEM ability to describe experimental track radii is seen in Fig. 2.

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