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Mathematical Modeling of Track Formation in $YBa_2Cu_3O_{7-x}$ Superconductor

B. F. Kostenko[*], **J. Pribiš**[†]
[*] *Laboratory of Information Technologies*
Joint Institute for Nuclear Research
Joliot-Curie 6, 141980 Dubna, Moscow region, Russia
[†] *Technical University in Košice*
Letná 9, 04001 Košice, Slovak Republic

Further development 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 within the framework of TEM.

Key words and phrases: track, accelerated ion, high-temperature superconductor, thermal spike, superheating, thermal explosion, model, computation.

1. Introduction

Nanodimensions 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, no satisfactory theory of track formation for these materials exists so far. Although different mechanisms were suggested till now, thermal spike and thermal explosion models were demonstrated to be most matchable for this purpose (see [1–3] 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 (in its traditional sense), existence of the electronic quenching phenomenon which results 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 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.

2. Thermal Spike and Thermal Exposion Models

In the thermal spike model (TSM), the following system of two coupled nonlinear differential equations for electron, T_e, and atom, T_i, temperatures is assumed:

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

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

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Parameters of the model were extracted from different independent experiments employing existing theory [2]. Initial conditions are chosen in a form

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

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.

TEM uses different description of melting process, although the same system of equation, (1) and (2). It takes into account a possibility of almost synchronous volumetric electron-atom energy transfer. In TSM, melting is described as loss of structural order in a thin layer near interphase boundary which gradually expands from the track center outside. 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.

3. Description of Energy Deposition

We developed a model of energy source, $q(r,\varphi,t)$, included in right side of equation (1), more exact than those usually used in calculations of this type. Namely, the space-time distribution of energy deposition upon electrons, accounting for its dependence on the projectile velocity, was simulated. The corresponding code (in FORTRAN) and its description is available [4]. It is in agreement with SRIM code [5] within 25 % accuracy (the precision of SRIM code itself is believed to be about 15 %). Radial distribution of dose around the path of a heavy ion matches the delta-ray model [6] of track structure, which is widespread in radiation dosimetry, within 10 % precision, and the δ-electron dynamics, suggested in [7], was used to find a time dependence of energy deposition at a given point, r, around the center of track.

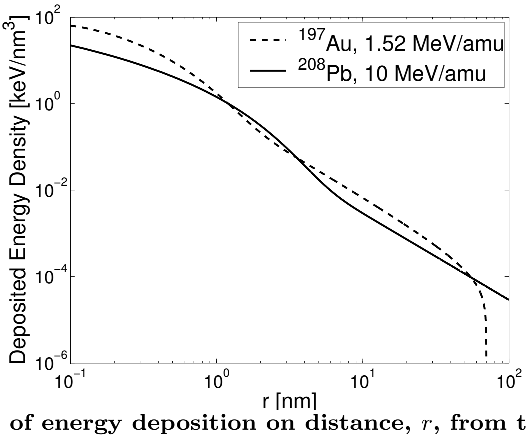

Figure 1. **Dependence of energy deposition on distance, r, from the center of track in $YBa_2Cu_3O_{7-x}$ for two different bombarding ions having nearly the same energy deposition per unit of ion's path, $dE/dx = 43.7$ and 44.1 keV/nm for Pb and Au, accordingly**

An example of calculations in the frame of this model is shown in Fig. 1, where two different ions with approximately equal stopping power, dE/dx is considered. The so-called velocity effect is seen as lower and wider distribution of energy deposition (in the range not very far from the track center) for a faster ion, as it was described in [8].

4. Mathematical Pecularities of TSM

It should be noted that the Stefan condition, often assumed when a moving surface of phase transition is formed, can not be accepted [9], before the energy source $q(r,\varphi,t)$ in (1) is turned off. Indeed, according to Stefan's condition, the following equation

$$K_{sol}\frac{\partial T(x_S+0,t)}{\partial x}-K_{liq}\frac{\partial T(x_S-0,t)}{\partial x}=L\rho_{sol}V_S,$$

defining Stefan's problem, is suggested (in this section a notation $T=T_i$ is introduced for short). Here V_S is the velocity of the boundary surface, K_{sol} and K_{liq} are thermal conductivities of the material for solid and liquid phases, L and ρ_{sol} are the melting heat and density, correspondingly. This simple balance is broken when energy deposition inside the region swept by the moving surface takes place. To overcome this difficulty, a generalized formulation of the Stefan problem suggested by A.N. Tikhonov and A.A. Samarskii [10],

$$(\rho C+L\,\delta(T-T^*))\frac{\partial T}{\partial t}=\mathrm{div}\,(K\ \mathrm{grad}\ T)+q(\mathbf{x},t).$$

was used. Here the term $L\,\delta(T-T^*)\ \partial T/\partial t$, describing the additional heat input expended on the phase transformation, is suggested to treat as an additional component of the thermal capacity which gives contribution only at the point of phase transition.

Another important feature of TSM is a sudden change of theoretical track radius, r_{th}, due to small alterations of D_e found for ^{129}Xe bombarding $YBa_2Cu_3O_{7-x}$ at 10 Mev/amu [2]. Numerical experiments shown this instability is caused by a transition from electronic heating of atomic subsystem to electronic quenching of it at the moment of formation of track boundary. Namely, for this ion electron temperature, T_e, becomes lower than the melting temperature at the moment when the melting region radius mounts to its upper value. For other ions or other initial energies, $r_{th}(T_e)$ dependence turned out to be also very strong although not so dramatic.

5. Properties of Electron Subsystem

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 [1–3]). The only unknown value the thermal diffusivity in $YBa_2Cu_3O_{7-x}$ as function of electron temperature was found via minimization of deviation of the theoretical track radii from experimental ones, is shown in Fig. 2. It satisfies the requirement to be $\simeq 1$ cm^2/s at high temperatures, as it was predicted in [11,12], and demonstrates a monotonous growth at $T_e > 10^4$ K, in qualitative agreement with [13]. 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

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

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[1] It was impossible to indicate an exact place where the value of $D_e(T_e)$ in Fig. 2 decreases essentially as far as electron temperature in a large region around track is much higher than T_0 at the moment of track boundary formation.

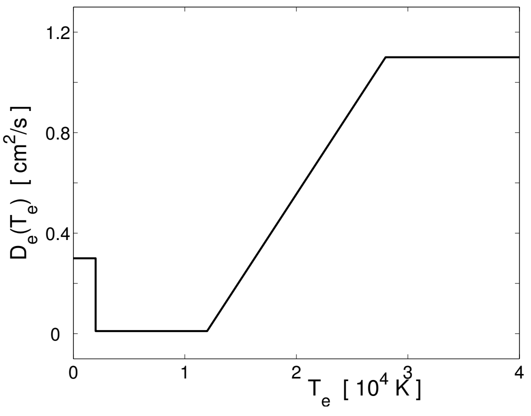

Figure 2. **Thermal diffusivity in $YBa_2Cu_3O_{7-x}$ as function of electron temperature, T_e, found from the requirement imposed on TEM to account for experimental track radii**

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

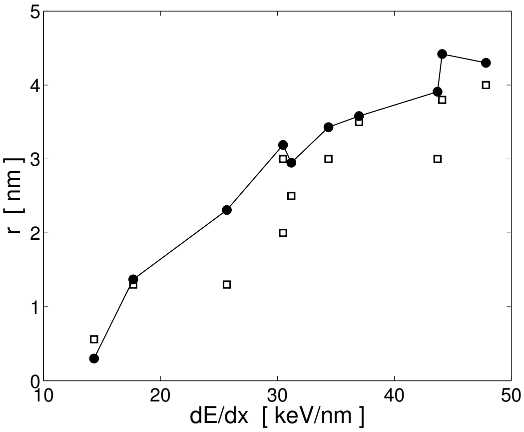

Figure 3. **Experimental (squares) and theoretical (circles) track radii obtained in the TEM framework for different ions bombarding $YBa_2Cu_3O_{7-x}$**

One can judge on the ability of TEM to describe experimental track radii using Fig. 3.

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Математичекое моделирование трекообразования в сверхпроводнике $YBa_2Cu_3O_{7-x}$

Б. Ф. Костенко*, Я. Прибыш†

* *Лаборатория информационных технологий*
Объединённый институт ядерных исследований
ул. Жолио-Кюри, д.6, Дубна, Московская область, 141980, Россия
† *Технический университет Кошице*
ул. Летна, д.9, Кошице, 04001, Словакия

Предложено дальнейшее развитие модели термовзрыва, описывающей трекообразование в высокотемпературных сверхпроводниках. Получена информация о температурной зависимости электронной температуропроводности в $YBa_2Cu_3O_{7-x}$ путем решения обратной задачи воспроизведения радиусов треков в рамках модели термовзрыва.

Ключевые слова: трек, ускоренные ионы, высокотемпературный сверхпроводник, термический пик, перегрев, термовзрыв, модель, вычисления.