Program for Calculation of Energy Deposition in Tracks of Charged Particles

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A program for calculation of radial energy distribution released in the vicinity of accelerated ions passing through the substance, accounting for the space-time dynamics of the process, were elaborated.

The radial distribution of dose around the path of a heavy ion can be calculated on line with the delta-ray model of track structure, which is widespread in radiation dosimetry [1]. The model incorporates energy deposition due to primary excitations and ionization of atoms, and δ-electron kinetic energy transfer. According to it, the primary excitations contribute essentially, about 50%, in the region r $<$ 10 nm. For r $>$ 10 nm investment of δ-electrons entirely dominates. Energy expended on ionization is taken into account using some mean ionization potential, of about 10 eV, which is subtracted from δ-electron kinetic energy. The stopping power calculated as the radially integrated dose distribution is in agreement with SRIM code [2] predictions within 25 % accuracy (the precision of SRIM code itself is believed to be about 15 %).

The radial distribution of dose cannot be regarded as instantaneous at least for t $\geq$ 10 fs when the thermal diffusivity of excited electron, $D_e \sim 1$ cm^2/s, should be taken into account. Further development of the delta-ray model in the required direction was undertaken in [3], where dissipation of the energy stored up in δ-electrons was described.

Thus, the space-time distribution of energy deposition, including its dependence on the projectile velocity, can be taken into account at least for $t > 10$ fs and $r >$10 nm, when δ-electron kinetic energy contribution to energy deposition utterly prevails.

For $t < 10$ fs the δ-electron dynamics can also be used as a rough approximation. One can ignore this inaccuracy since it is compensated by the time necessary for decays of primary excitations via the Auger transitions. Indeed, the most part of energy spent on track creation is released within the region $r < 1$ nm and $t < 0.15$ fs, although the process persists up to t $\sim 10^{-5}$ s and $r \sim 10^{-3}$ cm [3]. Calculations show that δ-electron energy deposition at r $<$10 nm comes to the end by the time of $t \sim 10$ fs. On the other hand, just by this moment Auger decays of all vacancies in the electron shells are expected to occur and thermodynamic equilibrium for the excited electrons to be established. Therefore, exactly the moment $t \simeq 10$ fs should be considered as a proper initial time, when the basic equations of thermal spike and thermal explosion models [4, 5] may be used in a consistent manner with the radial distribution of dose at that moment estimated by the simple δ-electron dissipation dynamics.

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

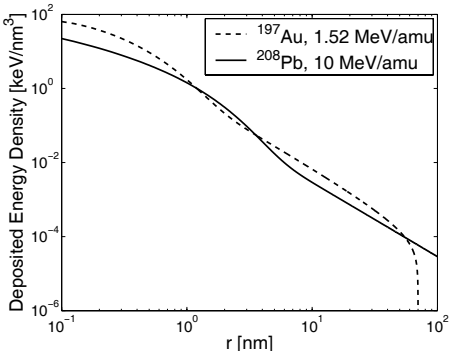

Figure 1: Dependence of energy deposition on distance, r, from the center of track in $YBa_2Cu_3O_{7-x}$ for two different bombarding ions having nearly the same energy deposition per unit of ion's path, $dE/dx = 43.7$ and 44.1 keV/nm for Pb and Au, accordingly

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 [6]. One can readily understand the phenomenon, as far as the faster ion is able to impose electrons more initial velocity and, therefore, push them further away from the center of track.

The corresponding code (in FORTRAN) and its description is available [7].

References

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