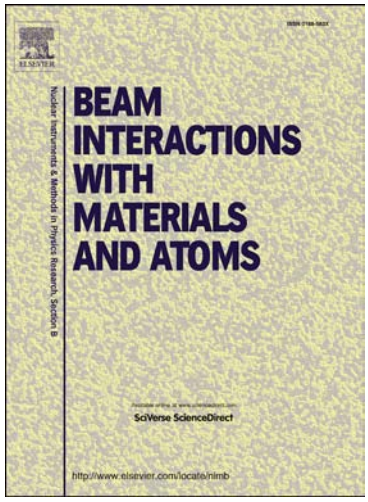

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S.A. Gorbunov, P.N. Terekhin, N.A. Medvedev, A.E. Volkov

PII: S0168-583X(13)00679-4
DOI: http://dx.doi.org/10.1016/j.nimb.2013.04.082
Reference: NIMB 59633

To appear in: *Nucl. Instr. and Meth. in Phys. Res. B*

Received Date: 29 November 2012
Revised Date: 29 April 2013
Accepted Date: 29 April 2013

Please cite this article as: S.A. Gorbunov, P.N. Terekhin, N.A. Medvedev, A.E. Volkov, Combined model of the material excitation and relaxation in swift heavy ion tracks, *Nucl. Instr. and Meth. in Phys. Res. B* (2013), doi: http://dx.doi.org/10.1016/j.nimb.2013.04.082

Combined model of the material excitation and relaxation in swift heavy ion tracks

S.A.Gorbunov[1], P.N.Terekhin[2], N.A. Medvedev[3], A.E. Volkov[1,2,4]

[1] LPI of the Russian Academy of Sciences, Leninskij pr., 53,119991 Moscow, Russia

[2] National Research Centre „Kurchatov Institute', Kurchatov Sq. 1,

123182 Moscow, Russia

[3] CFEL at DESY, Notkestr. 85, 22607 Hamburg, Germany

[4] JINR, Joliot-Curie 6, 141980 Dubna, Moscow Region, Russia

Abstract

A multiscale approach describing material excitation in the nanometric track of a swift heavy ion (SHI) decelerated in a solid in the electronic stopping regime is presented. This model consists of a combination of three different methods: (a) Monte Carlo simulations of excitation of the electron subsystem of a solid at the femtosecond scale due to scatterings of a SHI and generated fast electrons; (b) a molecular-kinetic approach describing the spatial spreading of electrons after finishing of ionization cascades up to timescales of a hundred femtoseconds; and (c) molecular dynamics simulations of reaction of the lattice on the excess energy transferred from the relaxing electron subsystem at the picosecond time scale. The Dynamic Structure Factor (DSF) formalism links together all these methods. It takes into account effects of spatial and temporal correlations in the atomic system of a target during its interaction with excited electrons in an ion track. For LiF crystals a good agreement is demonstrated between track heating estimated from the experimental data and that predicted by the model.

Keywords: swift heavy ion track, dynamical structure factor, molecular dynamics, Monte-Carlo, electron-lattice coupling

PACS: 72.10.−d, 11.80.La, 72.15.Lh, 72.20.Jv, 61.80.-x, 05.10.Ln, 52.65.Yy

*) a.e.volkov@mail.ru