Swift Heavy Ion Tracks in $Gd_2Ti_2O_7$ Pyrochlore: Effect of Electronic Energy Loss*

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Pyrochlore oxides ($A_2B_2O_7$) have recently been studied in detail with respect to their response to swift heavy ion irradiation. Characterization using complementary analytical techniques revealed a complex track-damage morphology consisting of an amorphous core surrounded by a disordered, defect-fluorite structured shell. Molecular dynamics (MD) simulations based on the inelastic thermal spike model were performed in which the time and temperature evolution of individual tracks is followed [1]. In order to provide further experimental insights into the formation of concentric nanoscale damage zones, the influence of the electronic energy loss dE/dx of GeV ions is investigated in gadolinium-titanate pyrochlore [2].

Polycrystalline samples of $Gd_2Ti_2O_7$ were polished down to 40 µm and irradiated with ^{58}Ni, ^{101}Ru, ^{129}Xe, ^{181}Ta, and ^{197}Au ions at the UNILAC accelerator with a specific energy of 11.1 MeV/u. The ions passed completely though the samples. The applied fluence of 5×10^{10} ions/cm^2 was low enough to avoid extensive track overlapping. The irradiated samples were crushed to a fine powder and investigated by means of high-resolution transmission electron microscopy (HR-TEM).

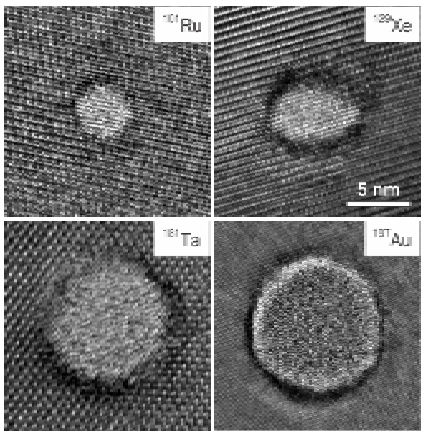

Figure 1: Cross-sectional HR-TEM images of cylindrical ion tracks in $Gd_2Ti_2O_7$ displaying a core-shell damage morphology. The dE/dx of the respective ions is 21.7 (Ru), 28.5 (Xe), 37.0 (Ta), and 40.1 (Au) keV/nm.

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The track damage is characterized by a core-shell structure (Fig. 1) changing from a defect-fluorite dominated shell at low dE/dx to predominantly amorphous tracks at high dE/dx. From Ru to Au ions, the amorphous fraction increases from 11 to 67% (Fig. 2) following an exponential growth with dE/dx, while the respective overall track diameter increases by about a factor of two (Fig. 2).

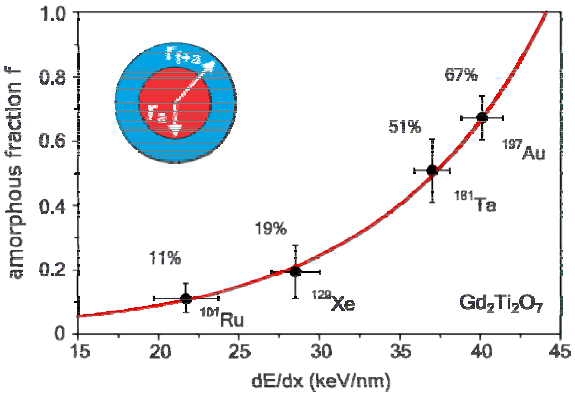

Figure 2: Amorphous fraction f of tracks in $Gd_2Ti_2O_7$ as a function of energy loss. f is estimated by the area ratio of the amorphous core (radius r_a) to the full track (radius r_{f+a}). The errors represent the dE/dx variation throughout the sample thickness, and the uncertainties of determining the area of amorphous core and entire track, respectively.

The size increase of tracks is primarily due to an expanding amorphous core, while the defect-fluorite structured shell radius remains almost constant. Thermal-spike calculations show that the molten track cross section increases with the energy deposition of the ions [2]. MD simulations reveal that the track shell results of a crystallization process from the track melt [1]. Thus, the shell thickness may be limited kinetically by material dependent crystallization front velocities. However, thermodynamic constraints on stabilization of a non-equilibrium phase may also contribute.

References

[1] J.W. Wang, M. Lang, R.C. Ewing, and U. Becker, *J. Phys.: Condens. Matter* 25 (2013) 135001.

[2] M. Lang, M. Toulemonde, J.M. Zhang, F.X. Zhang, C.L. Tracy, J. Lian, Z.W. Wang, W.J. Weber, D. Severin, M. Bender, C. Trautmann, R.C. Ewing, to be submitted (2013).