Multi-scale simulation of structural heterogeneity of swift-heavy ion tracks in complex oxides

JIANWEI WANG*, MAIK LANG, RODNEY C. EWING AND UDO BECKER

Department of Earth and Environmetnal Sceinces, University of Michigan, Ann Arbor, Michigan 48109 USA (*correspondence: jwwang@umich.edu)

Understanding and prediction of the phase behavior of materials under extreme environments provide a great challenge in the materials' design and engineering in various applications. Swift heavy ion have been used to probe the effect of the high-energy radiation on a wide variety of materials and to explore the complex far-from-equilibrium behavior of the materials under extreme conditions. In this study (J. Phys.: Condens. Matter,25,135001), track formation caused by a swift-heavy ion irradiation, 2.2 GeV Au, of isometric $Gd_2Ti_2O_7$ pyrochlore and orthorhombic Gd_2TiO_5 phase was modeled using thermal-spike model combined with a subsequent molecular-dynamics simulation. The thermal-spike model was used to calculate the energy dissipation over time and space. Using the time, space, and energy profile generated from the thermal-spike calculation, the molecular-dynamics simulation was performed to model the atomic-scale evolution of the track. The advantage of combining these two methods, that is using the output from the continuum model as an input for the atomistic model, is that it provides a means of simulating the coupling of the electronic and lattice subsystems and at the same time providing atomic-scale details of the track structure and morphology.

The simulated internal structure of the track consists of an amorphous core and a shell of disordered, but still crystalline, domains. For $Gd_2Ti_2O_7$, the shell region has a disordered pyrochlore with a defect fluorite structure and is relatively thick and heterogeneous with different degrees of disordering. For Gd_2TiO_5, the disordered region is relatively small as compared with $Gd_2Ti_2O_7$. In the simulation, "facets", that is surfaces with a definite crystallographic orientation, are apparent around the amorphous core and were more evident in Gd_2TiO_5 along the [010] than [001], suggesting an orientationally dependent radiation response of this structure. These results show that track formation is controlled by the coupling of several complex processes, involving different degrees of amorphization, disordering, and dynamic annealing. Each of the processes depends on the mass and energy of the energetic ion, the properties of the material, and its crystallographic orientation with respect to the incident ion beam.

Gallionella-like microorganisms involved in iron oxide formation in groundwater wells across a broad pH range

JUANJUAN WANG[1], MAREN SICKINGER[2] AND KIRSTEN KÜSEL[3]

[1]Friedrich-Schiller-University of Jena, Dornburgerstr.10 07743 Jena,(juanjuan.wang@uni-jena.de
[2]maren.sickinger@uni-jena.de
[3]kirsten.kuesel@uni-jena.de)

Clogging caused by iron ochre incrustations has been a challenge for the functioning of groundwater wells, especially technical wells in mining areas. The formation and dissolution of iron oxides can be mediated by iron-oxidizing and -reducing microorganisms. In this project we studied the potential role of these microbes in the clogging process at three locations in an open-cast mine, comparing a total of 16 wells. The groundwater had pH ranging from acidic (4.5) to neutral (7.5) and relatively high contents of Fe(II) (0.5~7 mM) and DOC (1.4~12.6 mgL^{-1}) at an average oxygen concentration of 3.8 mg $L^{-}1$. The mineral composition of ochres differed with ferrihydrite being common in circumneutral wells and schwertmannite dominating in the slightly acidic wells. 454 pyrosequencing revealed a high diversity of bacteria in the ochres with a large fraction of *Gallionella*-related sequences. Quantitative PCR suggested that *Gallionella*-related organisms on average accounted for 44 % of the total bacteria. Surprisingly, their abundance was not correlated to any geochemical parameter. *Gallionella*-related organisms were also present in the ground water ranging from 8.4×10^6 to 2.0×10^8 16S rRNA gene copies per L water. Iron reducing bacteria such as *Geobacter*, *Geothrix*, *Rhodoferax*, were only detected at low abundance, in agreement with a low iron reduction potential. However, the iron reduction potential could be stimulated by the addition of lactate. In conclusion, *Gallionella*-related iron oxidizers dominated ochres and groundwater irrespective of pH, suggesting a major role of these organisms in the formation of ochres across a broad range of geochemical conditions. Deeper insight into the microbiology of the ochre formation process may help to develop strategies for relieving clogging problems in technical wells.

DOI:10.1180/minmag.2013.077.5.23