Interactions between nitroaromatic (TNT) and nitramine (RDX) explosives and pure minerals

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We studied geochemical interactions between the explosives compounds TNT and RDX and common soil minerals. TNT and RDX are among the most widely used energetics on military training lands and an understanding of their fate in soils is key to effective range management. One kg. of 11 different pure mineral phases was proximally detonated with composition B, a mixture of TNT and RDX. Detonated and pristine minerals were investigated using x-ray diffraction, gas adsorption surface area measurements, scanning electron microscopy, and attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR). Batch slurries were created by mixing detonated or pristine minerals with deionized water and measuring concentrations of primary explosives and transformation products in solution for 100 days. Detonated samples generally exhibited lower gas adsorption surface areas than their pristine counterparts, perhaps from explosives residue coating, shock-induced compaction and/or partial fusion. TNT and RDX exhibited analyte loss in almost all batch solutions but analyte loss was greater in vermiculite, bentonite and biotite than in muscovite and quartz. ATR-FTIR measurements showed evidence of interactions between explosives nitro groups and mineral surfaces. A band position shift of the explosive nitro group peaks of TNT and RDX was observed for all minerals but was greater in vermiculite, nontronite and bentonite than in quartz. Our results suggest that range design or remediation options should include the use of specific mineral substrates to promote explosives transformation.

An experimental study of Fe isotope fractionation between silicate melt and spinel

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Fractionation of Fe in high temperature environments has been described in settings ranging from a lava lake undergoing magmatic differentiation [1] to mantle rocks from various terrains [2, 3]. It has been proposed that Fe fractionation is linked to its variable oxidation state [4]. Indeed, $\delta^{57/54}$Fe ratios in spinel and $\delta^{56/54}$Fe ratios of bulk basaltic rocks have been correlated with $Fe^{3+}/\Sigma Fe$ [1, 2]. Fe isotopes have therefore been suggested as a proxy for oxygen fugacity (fO_2) [2].

We aim to determine the extent of Fe isotope fractionation with Fe^{2+}/Fe^{3+} partitioning between phenocryst-basalt glass pairs in a series of samples synthetically created under known fO_2 conditions.

Whereas large Fe fractionations have been observed between olivine phenocrysts and basalt (the phenocrysts being up to 1.2 per mil (‰) lighter than basalt whole rock [1]), the olivine mineral structure precludes Fe^{3+} substitution, possibly limiting the potential for fractionation. In contrast, spinel ($A^{2+}B_2^{3+}O_4$) accommodates both Fe^{2+} and Fe^{3+}, potentially negating structural bias. Systematic variation in Fe isotope composition of spinels (on the order of 1.7 ‰ $\delta^{57/54}$Fe) has already been noted [2], further supporting its use in this study.

Synthetic samples with basaltic composition were prepared under a range of oxygen fugacities from NiNiO+3 to NiNiO-4, with chromite spinel as the only liquidus phase. As expected, major element compositions vary systematically with fO_2 (spinel ranging from $Mg_{0.6}Fe_{1.4}Cr_{0.8}Al_{0.5}O_4$ to $Mg_{0.4}Fe_{0.7}Cr_{1.4}Al_{0.5}O_4$). The glass and spinel have been separated by acid digestion. We shall report on Fe isotope measurements of the co-existing spinel and glass.

[1] Teng *et al*. (2008) *Science* **320**, 1620-1622. [2] Williams *et al.* (2004) *Science* **304**, 1656-9. [3] Wlliams *et al*. (2005) *EPSL* **235**, 435-452. [4] Weyer (2008) *Science* **320**, 1600-1601.