Structure and Radiation Damage in $Y_2Ti_2O_7$ and Y_2TiO_5

M. ROBINSON[1], N.A. MARKS[1]*, D.J. CARTER[1],
M.J. QIN[2], S.C. MIDDLEBURGH[2], G.J. THOROGOOD[2],
E.Y KUO[2], R.O. AUGHTERSON[2] AND G.R. LUMPKIN[2]

[1]Nanochemistry Research Institute, Curtin University, Australia (*correspondence: N.Marks@curtin.edu.au)
[2]Australian Nuclear Science & Technology Organisation, Locked Bag 2001, Kirrawee DC, 2232, NSW, Australia

Yttrium titanate is a rich solid-state system with important applications in a nuclear context. When it takes the stoichiometry $Y_2Ti_2O_7$ yttrium titanate adopts the pyrochlore form, a crystal structure which has been extensively studied as an immobilization matrix for nuclear waste. Y-Ti-O nanoparticles are also key ingredients in high-performance oxide-dispersion-strengthened (ODS) steels needed for next-generation fission and fusion reactors. The structure of these nanoparticles is complex and not fully clear, spanning a range of possibilities including enriched clusters, defective rocksalt-type TiO phases as well as stoichometric $Y_2Ti_2O_7$ and Y_2TiO_5 [1,2]. The Y_2TiO_5 structure itself is poorly understood, with the phase diagram thought to comprise a low-temperature orthorhomic phase, a high-temperature cubic phase, and a hexagonal phase at intermediate temperatures [2].

Here we develop a new interatomic potential for yttrium titanate and apply it to both the determination of structure and irradiation response. The potential employs partial charges and is fitted to lattice parameters, internal coordinates and elastic constants obtained from density-functional-theory. For both $Y_2Ti_2O_7$ and orthorhombic Y_2TiO_5 the potential provides a substantial improvement over existing literature models.

Recent experiments [3] have shown that cubic Y_2TiO_5 exhibits a pyrochlore-derived superstructure involving a tripling of the unit cell along 111 directions. To determine its structure, Monte Carlo simulations were performed to order the cations and anions within a large 3×3×3 tiling of the 88-atom unit cell. Experimental diffraction reflections were used to arrange the cations by calculating the structure factor, while the potential was used to order vacancies on the oxygen sub-lattice. The potential was also employed in Molecular Dynamics calculations of threshold displacement energies, thermal spikes and radiation damage cascades in $Y_2Ti_2O_7$ and Y_2TiO_5. Using these simulations we interpret experimental studies of amorphization and quantify the role of anti-sites and structure in radiation response.

[1] Hirata *et al.* (2011) *Nature. Mat.* **10**, 922-926. [2] Jiang *et al.* (2010) *Acta Mater.* **58**, 1536-1543. [3] Whittle *et al.* (2011) *Acta Mater.* **59**, 7530-7537.

A new model for the formation of podiform chromitites in ophiolites

PAUL T. ROBINSON[1]*, JINGSUI YANG[1], MEI-FU ZHOU[2]
AND FAHUI XIONG[1]

[1]Chinese Academy of Geological Sciences, Beijing, China (*correspondance: paulrobinson94@hotmail.com)
[2]Department of Earth Sciences, Univ.of Hong Kong, Hong Kong, SAR, China (mfzhou@hku.hk)

Podiform chromitites occur in the upper mantle sections of ophiolites where they are typically surrounded by dunite envelopes formed by melt-rock reaction. Both high-Cr and high-Al varieties are common, but rarely in the same ophiolite. In contrast, residual chromite grains in the host peridotites and dunites show a wide range of composition. The podiform chromites are generally thought to be magmatic precipitates from suprasubduction (SSZ) melts migrating through the mantle wedge However, the recent confirmation of diamonds in both podiform chromitites and peridotites of several ophiolites, and evidence suggesting depths of formation >300 km for some of the chromites, challenges this model. All UHP minerals would be destroyed if they were exposed to SSZ melts at shallow mantle levels. We suggest that residual chromites first crystallize as discrete grains in mantle peridotites beneath mid-ocean spreading centers near the top of the transition zone, where they encapsulate diamonds and highly reduced phases carried by fluids from greater depths. These would be high-Al chromites, indicating relatively low degrees of partial melting of the host peridotites. Some of these chromite-bearing mantle sections in which diamonds occur are eventually trapped in suprasubduction zones where they are infiltrated by hydrous SSZ melts, either arc tholeiitic or boninitic in composition. As these melts migrate through the mantle wedge they react with the host peridotites, dissolving pyroxene, precipitating olivine in dunite ‘channels’, and becoming progressively enriched in Cr. These melts react with and locally remobilize the ‘residual’ chromite grains, increasing their Cr#. The residual chromite grains are not melted but become more Cr rich by diffusion. The remobilized chromite grains are carried to shallow levels by the rising melts where they are deposited, along with newly precipitated grains, as podiform chromitites. The UHP minerals within the chromite grains are not destroyed because they are protected from the melts. This model accounts for the fact that podiform chromitites are found only in ophiolites and for the preservation of UHP minerals in both podiform chromitites and residual chromites within the host peridotites.

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