Metamorphism and *P-T* evolution of high pressure granulite in Chicheng, Northern part of the paleoproterozoic Trans-North China Orogen

DINGDING ZHANG AND JINGHUI GUO

Institute of Geology and Geophysics, Chinese Academy of Sciences, Beijing 100029, China (correspondence: zhangdingdingx @163.com)

It is widely accepted that the North China Craton formed by collisional amalgamation of the Eastern and the Western Blocks along the central Trans-North China Orogen (TNCO) at ~1.85 Ga. However, the continental subduction process has not been well recorded by previously reported high-pressure (HP) granulites due to lack of prograde metamorphism because of high peak temperature. Recently, we have identified a set of HP mafic granulites with well preserved prograde metamorphism in the Womakeng of ChiCheng, northern part of the TNCO. They developed among a granulite facies mafic to felsic metavolcanic rock association. The prograde metamorphic stage (M1) has been revealed by distinct growth zone of garnet porphyroblasts with inclusion rich core and inclusion free mantle. The peak metamorphic mineral assemblage (M2) consists of Grt and Cpx predominantly with minor Pl, Rut, Amph and Qtz. The Pl+Amph symplectite or corona surrounding garnet and Cpx+Ilm symplectite arround titanite documented the post-peak decompression (M3) stage. Phase equilibria modelling by THERMOCALC software yielded a consecutive clockwise *P-T* path with a remarkable prograde metamorphic section, during which the tempretures increase from 630~680 ℃ to 700~750 ℃ as coincident increase of pressures from 9~11 kbar to the peak (14~16 kbar). During decompression after peak from 16 kbar to 10 kbar, the temperature keeps increasing from 700~750 ℃ to 750-800 ℃ indicating a thermal relaxation, and then decreases as the pressure further descends. The new defined *P-T* path of the HP granulites provide a better metamorphic evidence for the subduction process during the continental collision along the Trans-North China Orogen.

The effect of chemical evolution in ^{137}CsCl on radionuclide leaching

F. ZHANG[1], N. A. MARKS[1], J. D. GALE[1], Q. KANG[2],
B. P. UBERUAGA[2], C. R. STANEK[2] AND N. HENSON[2]

[1]Nanochemistry Research Institute, Curtin University,
PO Box U1987, Perth, Western Australia 6845, Australia
[2]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

A critical component of nuclear waste disposal strategy is to prevent radionuclides from leaving the waste form and entering the environment. However, radiation damage and leaching studies over the past 30 years have focused on the performance of the candidate waste form at t=0, with far less attention paid to the phase stability, and subsequent durability, during the course of daughter product formation. As a case study in chemical aging, we consider here the system of ^{137}CsCl, capsules of which exist in storage pools at Hanford, Washington State. We combine density-functional-theory (DFT) calculations with pore sale modeling to gain a sense of how radionuclide leaching varies as a function of time due to in-growth of the daughter products.

In previous calculations of bulk material we have shown [1,2] that beta-decay of ^{137}Cs to stable ^{137}Ba generates a rocksalt BaCl daughter phase in which the Ba does not have the expected 2+ oxidation state. This phenomenon is an example of a process we term radioparagenesis [3], in which decay of a major lattice constituent gives rise to a novel solid state daughter phase. Here we study radioparagenesis at surfaces, finding that isolated Ba atoms are most stable in the sub-surface layer, while pairs of Ba atoms have a large binding energy. The Ba atoms also enhance segregation of Cs and Cl vacancies to the surface, suggesting that although Ba will not easily migrate to the surface of the crystal, it significantly modifies the behavior of other defects. In particular, when water interacts with the CsCl surface, the dissolution energy will depend on whether there is Ba nearby or not. Using Schottky defect formation energies derived from DFT, pore-scale modelling simulations were used to predict dissolution of CsCl into water at 20 °C. The models show that the CsCl leaching rate significantly increases when Ba is present, suggesting that chemical aging should be considered as an additional factor in waste form design.

[1] Jiang *et al.* (2009) *Phys. Rev. B* **79**, 132110. [2] Uberuaga *et al.* (2010) *Nucl. Instrum. Meth. B* **268**, 3261-3264. [3] Jiang *et al.* (2010) *Energy & Environ. Science* **3**, 130-135.

DOI:10.1180/minmag.2013.077.5.26