A mineral record of 4.0Ga metamorphism: Evidence of metamorphic zircon xenocryst from western North Qinling Orogenic Belt

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One zircon xenocryst with a concordant 207Pb/206Pb age of 4079±5Ma was determined by Wang [1] from Ordovician volcanic rocks. This zircon age has been the oldest one reported in the Qinling Orogenic Belt and was interpreted as the zircon crystallization age. Sun [2] also recognized some ~3.5 Ga old magmatic zircon xenocrysts from the same area. These zircon grains obviously have negative εHf(t) values and Hf model ages ranging from 3.8 Ga to 4.0 Ga, suggesting that their source rocks were may have come from recycled Paleoarchean crust. The host rocks contain Hadean zircons are clearly defined as pyroclastic lava, not volcanic lava, as previously believed.

Recently, about 3,000 zircon grains collected from the same rock suite have been analyzed by LA-ICPMS. One zircon xenocrystic core gave a concordant 207Pb/206Pb age of 4008 ± 29 Ma. The zircon has a clear core-rim structure with a dark core in CL image and a Th/U ratio of 0.04, indicating characteristics of metamorphic zircon (Fig.1) Combining the above data, our discovery provides strong evidence for the existence of ~4.0 Ga old crustal relics in the North Qinling Orogenic Belt..

Based on the large amount of study on the petrogenesis of zircon, the earliest magmatic event on the Earth has been inferred to occurred over the period from 4.4 to 3.9 Ga [3-4]. However, our study have provided an evidence that the metamorphic event could occurred as early as 4008 Ma ago,
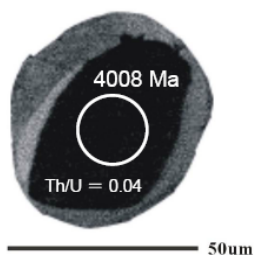

Although it's unknown what kind of metamorphic environment was involved in formation such zircon, Nevertheless, the occurrence of 4.0 Ga metamorphic zircon indicates that the mass of continental crust was largely established in the Early Archean, maybe as far back as ca. 4400 Ma.

Figure 1: Zircon CL image

[1] Wang et al. (2007) Chin Sci Bull **52**, 3002-3010. [2] Sun et al. (2008) GCA **72**(12), A916. [3] Cavosie, (2005) EPSL **235**, 663–681. [4] Nemchin et al. (2006) EPSL **244**, 218–233

Computational studies of geochemical processes: CO_2 sequestration, metal ion solvation, and isotope fractionation factors

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Advances in theory, algorithms, software, and computer architectures, have made it possible to calculate reliably the thermodynamics and, in some cases, reaction kinetics for geochemical processes in solution. The capture and storage of the green house gas CO_2 in deep geologic formations represents one of the most promising options for mitigating the impacts of greenhouse gases on global warming owing to the potentially large capacity of these formations and their broad regional availability. We will describe computational studies of the reactions of CO_2 in water clusters to model aqueous systems using reliable computational approaches, CCSD (T) with large basis sets and self consistent reaction field (SCRF) approaches to model the extended solvent. We have extended these studies to models of wet supercritical CO_2 by investigating the properties of water molecules in CO_2 clusters. The results show the importance of Lewis acid-base interactions over hydrogen bonding. Such studies are critical to modelling the reactions of CO_2 injected into subsurface sequestration systems to determine their effects on the actual storage system, for example pore clogging or caprock fracturing. We are also studying the properties of aqueous metal ions as their interactions will be important in determining the subsurface chemistry of CO_2. We have found that for the +2 metal aquo ions it is possible to predict the size of the first solvation shell by predicting the correct pK_a in terms of experiment. The calculations are done at the MP2 level with large basis sets and SCRF approaches. They show that it is possible to predict pK_a's to better than 1 pK_a unit in most cases with pK_a's ranging from ~-5 for UO_2^{2+} to ~10 for many transition metal ions. As an example, high level calculations and HEXS experiments on UO_2^{2+} have shown that there are 4 to 5 H_2O molecules in the first solvation shell. The best agreement with experiment for the predicted pK_a (UO_2^{2+}) is found with 5 H_2O molecules. Poor agreement was found for 3+ and 4+ metal ions suggesting that the larger positive charges require more solvation shells due to the charge delocalization beyond the first solvent shell. Isotope fractionation factors for carbonates will also be discussed.