

Zinc incorporation into hydroxylapatite

YUANZHI TANG^{1,3}, RICHARD J. REEDER¹
AND YOUNG J. LEE^{2*}

¹Department of Geosciences and Center for Environmental Molecular Science, Stony Brook University, Stony Brook, NY 11794-2100, USA (ytang@seas.harvard.edu, rjreeder@notes.cc.sunysb.edu)

²Department of Earth and Environmental Sciences, Korea University, Seoul 136-701, Korea
(*correspondence: youngjlee@korea.ac.kr)

³Present address: School of Engineering and Applied Sciences, Harvard University, 40 Oxford St., Cambridge, MA 02138, USA

Zn substitution in apatite-like materials has been the focus of many studies because of its presence in all biological tissues and diverse roles in biological functions, including calcification. The uptake and release of Zn in the body is strongly mediated by the bone reservoir, even though it only contains a small portion of the total body Zn. The presence of Zn in teeth has been used as an indicator of environmental exposure. Yet, the mode of Zn incorporation into hydroxylapatite, specifically the binding site and its local structure, is still not clearly understood. The main uncertainties arise due to the presence of two structurally distinct cation sites and the potential for different Zn coordination geometries (tetrahedral and octahedral).

Results of theoretical modelling and X-ray absorption spectroscopy have been used to evaluate the local coordination structure of Zn incorporated into hydroxylapatite. Density function theory (DFT) calculations show that Zn favors the Ca2 site over the Ca1 site, with a preference for tetrahedral coordination. X-ray absorption near edge structure (XANES) spectroscopy suggests one dominant coordination environment for Zn, and no evidence was observed for other Zn-containing phases. Extended X-ray absorption fine structure (EXAFS) fitting of the synthetic samples confirms that Zn occurs in tetrahedral coordination at the Ca2 site, with two P shells at ~2.85–3.07 Å, and two Ca shells at ~3.71–4.02 Å. These fit results are consistent with the most favored DFT model for Zn substitution in the Ca2 site. The tetrahedral coordination requires local disruption of the structure. The results provide the structural basis for future models of Zn uptake and exchange in apatite-like biomaterials.

Fast reduction of U-Pb data using R

M. TANNER* AND L. SOLARI

Centro de Geociencias, UNAM, 76230, Santiago de Querétaro, Mexico (*correspondence: m.tanner@gmx.ch)

U-Pb data of Laser Ablation Inductively Coupled Plasma Mass Spectrometry

Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) provides fast and reliable U-Pb dating of minerals like Zircons. Careful treatment of raw data is key to get reproducible results.

Our script 'Upb.age' for R, a free software environment for statistics and graphics, provides functionality to read and process series of measurement files. Measured standard materials are recognized by the measurement names. User defined integration windows are used for gas blank correction of the signals. Possible inclusions and outliers are detected with a robust regression model and presented to the user for exclusion or to redefine the corresponding signal integration window. Instrument drift can be included in correction factors based on data of a linear model of the standard measurements. Age relevant isotope ratios are calculated from average ratios. Alternatively down-hole fractionation can be addressed by using the x-axis intercept of a linear model through the individual time related ratios [1]. For samples with reduced integration window correction factors are recalculated applying this new window on all standard measurements. The results are saved in comma separated value (CSV) format and can directly be evaluated by the Excel addin Isoplot [2].

The provided functionality is currently optimized for a 193 nm excimer laser ablation system coupled to an ICP-quadrupole-MS. Therefore a common lead correction is not provided but data for mathematical correction following Anderson [3] is included in the result file.

[1] Horn *et al.* (2000) *Chem. Geol.* **164**, 281-301. [2] Ludwig (1980) *Earth Planet. Sci. Lett.* **46**, 212-220. [3] Andersen (2002) *Chem. Geol.* **192**, 59-79.