Hydrous and anhydrous metal formates – Properties and applications

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Synthesis and Results

The metal formate hydrates are synthesized by reaction of metalcarbonate, metalhydroxide or metaloxide and formic acid in an aqueous solution. The crystallisation process takes place at a temperature of 20°C.

The characterisation of the crystals was done by X-ray diffraction, thermogravimetry, scanning electron microscopy and Karl-Fischer-titration.

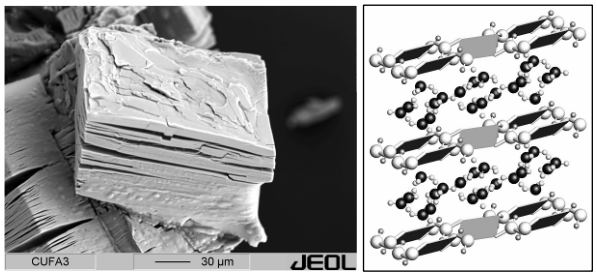

Figure 1: SEM image of $Cu(HCOO)_2$, dehydrated from $Cu(HCOO)_2 \cdot 4H_2O$ at 20°C and the crystal structure

Discussion

It is impotant to investigate the crystallographic properties of the formate and their stability to investigate in further experiments the effect on acceleration and retardation of formates as admixture in Ordinary Portland Cement. In addition, we investigate the dehydration and decomposition of the metal formate to produce particles in nanometer size. The metal carboxylate are suitable because of their low decomposition temperatures.

Conclusion

By using the crystallographic information of hydrous and anhydrous metal formates, theoretical predictions for applications are be obtained.

References

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Molecular dynamics simulations of fission track annealing in apatite

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Our aim is to use molecular dynamics simulations to elucidate how the composition of apatite minerals $Ca_{10}(PO_4)_6(F,Cl,OH)_2$ affects the annealing rate of the natural fission tracks, which form in the apatites as a result of the spontaneous fission of uranium. Knowledge of the effects that the many species present in natural apatites, particularly fluoride, chloride and hydroxide, have on the annealing rate is invaluable in interpreting accurately the results of fission track data for geothermochronometry.

The fission tracks formed by uranium fission in apatite are typically 14 µm long and 50 Å in diameter. The formation of tracks in apatite can be adequately modelled using a method where atom velocities are altered perpendicular to the track, which model produces tracks which are consistent with those obseved experimentally.

The simulations show that the diameters of tracks formed in two crystal directions are similar for a series of six apatites of different composition. In pure chlorapatite the simulated tracks are somewhat larger in both crystal directions, whereas in fluoride-bearing apatites small clusters of calcium fluoride are consistently formed in the track region.

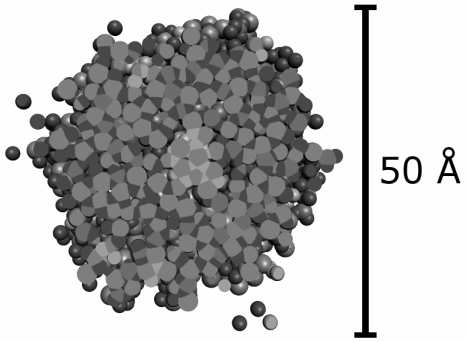

Figure 1: Disrupted atoms looking down a fission track.

Simulating the annealing of fission tracks is a great challenge for molecular dynamics because of the long timescales involved. We are currently developing a method to accelerate annealing by pulling atoms back to their equilibrium positions. The distributions of atomic transition energies from such simulations show some clear trends, in agreement with experiment, which suggest that the rate of annealing can be derived from short molecular dynamics simulations.