Poster Presentation

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On the formation of TiO2 nanocrystalites in HCl aqueous solution

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Pyrolysis of titanium tetrachloride (TiCl4) in HCl acidic aqueous medium shows that the HCl concentration in the synthesizing medium and the following aging are the essential factors affecting the phase formation and composition of the resulting TiO2 nanocrystals. The TiO2 suspended in the HCl medium is anatase in uniform cluster and the TiO2 deposited in the sedimentation is rutile in the rod-like structure. Consequnece, TiO2 nanocrystallites in pure anatase and rutile phase can be extracted and segregated from the colloidal suspension and the deposited parts in the synthesizing medium.
The formation of TiO2 nanostructures with different crystalline phases and morphology in HCl acidic aqueous medium is explained by two mechanisms: the dissolution and recrystallization mechanism and the in situ transformation mechanism. The formation of anatase in suspension part is likely belonging to the first mechanism and the formation of rutile in the sedimentation is belonging to the second mechanism. The first mechanism governs the formation of anatase and is proceeded by the second mechanism as a result of correlation between the free energy and the size limitation of TiO2 colloids in the solution. As a result of competition between the surface and bulk free energy, below a size limitation, the TiO2 rutile crystallites have higher free energy than that of the anatase and vice versa. Consequently, the resulting TiO2 in the solution is predominant anatase phase with size is below the limitation (10 nm), exceeding the size limitation the in situ anatase to ruttile transformation occurs and rutile crystallites at bigger size are formed and then deposited in the sedimentation. In the equilibrium condition, the smaller particles in the colloidal solution are predominant anatase, and the bigger nanoparticle will deposite at the bottom of the flask will be predominant rutile. The anatase to rutile transformation is enhanced by the present of HCl. A solvent environment with the presence of HCl creates Ti4+ ion converting solvent and the formation of TiO2 crystals, which makes the split of crystals in the anatase and rutile phase easier. During the TiO2 growth process, HCl worked like a chemical catalyst causing a change in crystallization and decreasing the activation energy for the rutile formation. By adjusting the HCl concentration, the rutile/anatase ratio is changed as the equilibrium condition is changing.
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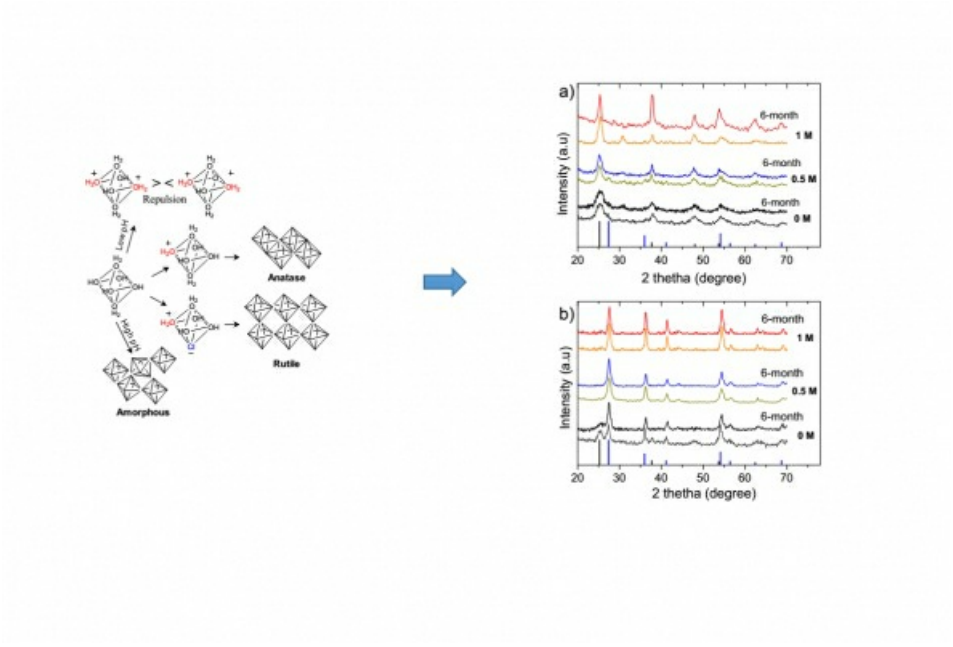

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