Dependence of Photocatalytic Activities on the Crystal Structure of Titanium(IV) Oxide Particles for Environmental Applications

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Anatase and rutile are predominant polymorphs of titanium(IV) (titania) and titania photocatalysts, widely used in environmental applications, are composed of each of them or their mixture. Their photocatalytic activity is often discussed in relation with these polymorphs, e.g., anatase is better than rutile. However, it is rather difficult in strict scientific sense to prove these hypotheses, because a pair of powder samples of completely same physical properties except for crystal structure can not be prepared and compared with each other. This study aims at clarifying the above-mentioned hypothesis through statistical analyses of physical properties and photocatalytic activity of 35 commercial titania samples.

Five test photocatalytic reactions were as follows: a) Oxygen (O2) liberation from a deaerated silver sulfate aq., b) Dehydrogenation of methanol in a deaerated water, c) Oxidative decomposition of acetic acid in an aerated aqueous solution, d) Oxidative decomposition of acetaldehyde in air, and e) Synthesis of pipelicolic acid (PCA) from L-lysine (Lys) in a deaerated aqueous solution. The standardized reaction rates were compared with each structural property, specific surface area (BET), density of lattice defects (DEF), primary particle size (PPS), secondary particle size (SPS), and existence of anatase (ANA) and rutile (RUT) phases. The data were analyzed statistically by solving a following matrix equation, [rate]_{35x1} = [property]_{35x6} \times [coefficient]_{6x1}, for each reaction.1)

Table 1 shows the results of analyses. As a general trend, reactions a) and e) gave relatively larger $R^2$s, i.e., higher reproducibility of the results, while those for the others were also fairly high. Another significant feature is that coefficient of $k_{ANA}$ has large positive value in all the cases except for reaction a). This is the first example supporting a general understanding that anatase is more active than rutile. On the other hand, $k_{RUT}$ was relatively small suggesting that rutile is rather inert compared with anatase. For reaction a), $k_{ANA}$ was small but positive, while $k_{RUT}$ was not so large, suggesting that rutile is not indispensable for higher activity. It seems that large secondary particles (large positive $k_{SPS}$) composed of large primary particles of less crystalline defects (negative $k_{DEF}$) are preferable as reported so far. A significant point is that the reported higher activity of rutile powders for reaction a) is mainly attributable to their secondary particle size, but not to rutile crystal.

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Recent Publications:


Biographical Sketch:

After obtaining a Bachelors degree at the Universidad Mayor de San Andrés in Bolivia in 2003, Orlando Prieto was awarded a Scholarship from the Japanese Government to pursue postgraduate studies at Hokkaido University in Japan. He completed his Masters course in 2006 and immediately enrolled into the Doctoral course, under the academic mentorship of Professor Bunsho Ohtani within the Graduate School of Environmental Earth Science, from which he will be graduating soon. His research focuses on the study of the interdependence between the structural characteristics of titania powders and their photocatalytic activity as a fundamental means for the design of high performance photocatalysts.