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REACTION KINETICS, CATALYSIS AND.....

碳纳米管及C_{60}和石墨氧化动力学机理函数的分析

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摘要 The oxidation of carbon nanotubes, C60 and graphite was studied by thermogravimetric (TG) analysis and differential thermal analysis (DTA) technique, and the oxidation kinetic models of three carbon materials studied were analyzed by mechanism-function method. The results indicate that three carbon species adopt different oxidation mechanisms due to their different structures. The oxidation of carbon nanotubes with cylindrical structure follows contracting volume reaction mechanism [R3 mechanism, 1- (1- α) ^1/3 = kt], indicating that the oxidation of carbon nanotubes takes place from the ends to the center. For graphite with planar sandwich structure, the oxidation starts at the edges initially and gradually moves toward the center, which corresponds to contracting area phase boundary reaction mechanism [R2 mechanism, 1 - (1 - α)^1/2 = kt]. The oxidation of C60 with spherical structure, however, is complex and apparently cannot be illustrated with a single kinetic model. The values of apparent activation energy obtained by the mechanism-function method are (145 ± 5) kJ·mol^-1 for carbon nanotubes and (193 ± 7) kJ·mol^-1 for graphite, respectively, while the value of apparent activation energy for C60 determined using Kissinger method is 91 kJ·mol^-1.

关键词 C60 碳纳米管 氧化作用 动力学分析 石墨

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Kinetic Analysis of Oxidation of Carbon Nanotubes, C60 and Graphite Using Mechanism-Function Method

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Abstract The oxidation of carbon nanotubes, C60 and graphite was studied by thermogravimetric (TG) analysis and differential thermal analysis (DTA) technique, and the oxidation kinetic models of three carbon materials studied were analyzed by mechanism-function method. The results indicate that three carbon species adopt different oxidation mechanisms due to their different structures. The oxidation of carbon nanotubes with cylindrical structure follows contracting volume reaction mechanism [R3 mechanism, 1- (1- α) ^1/3 = kt], indicating that the oxidation of carbon nanotubes takes place from the ends to the center. For graphite with planar sandwich structure, the oxidation starts at the edges initially and gradually moves toward the center, which corresponds to contracting area phase boundary reaction mechanism [R2 mechanism, 1 - (1 - α) ^1/2 = kt]. The oxidation of C60 with spherical structure, however, is complex and apparently cannot be illustrated with a single kinetic model. The values of apparent activation energy obtained by the mechanism-function method are (145 ± 5) kJ·mol^-1 for carbon nanotubes and (193 ± 7) kJ·mol^-1 for graphite, respectively, while the value of apparent activation energy for C60 determined using Kissinger method is 91 kJ·mol^-1.

Key words oxidation mechanism; carbon nanotubes; kinetic analysis; activation energy

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