9 References

[1] R. Feynman (1965) *The Feynman Lectures on Physics*, Vol. 3. Addison-Wesley, Reading.

[2] A.J. Arduengo, R.L. Harlow and M. Kline (1991) A stable crystalline carbene. *Journal of the American Chemical Society*, 113, 361–363.

[3] P. Atkins and J. de Paula (2002) *Atkins' Physical Chemistry*. Oxford University Press, Oxford.

[4] R. Bacon (1960) Growth, structure, and properties of graphite whiskers. *Journal of Applied Physics,* 31, 283–290.

[5] V.V. Korshak (1987) Electronic structure of carbynes studied by Auger and electron energy loss spectroscopy. *Carbon*, 25, 735–738.

[6] N.W. Ashcroft and N.D. Mermin (1976) *Solid State Physics*. Harcourt, Fort Worth, US.

[7] F.V. Chukrov, B.B. Zvyagin, A.P. Zhukhlistov, N.I. Organova and L.P. Yermilova (1986) Structural features of natural graphite. *International Geology Review*, 28, 790–801.

[8] G. Parthasarathy, B. Sreedhar and T.R.K. Chetty (2006) Spectroscopic and X-ray diffraction studies on fluid deposited rhombohedral graphite from the eastern Ghats Mobile Belt, India. *Current Science*, 90, 995–1000.

[9] S. Amelinckx, P. Delavignette and M. Heerschap (1965) Dislocations and stacking faults in graphite. In P.L. Walker (Ed.), *Chemistry and Physics of Carbon*, Vol. 1, Marcel Dekker, New York.

[10] J.M. Thomas (1965) Microscopic studies of graphite oxidation. In P.L. Walker (Ed.), *Chemistry and Physics of Carbon*, Vol. 1, Marcel Dekker, New York.

[11] C. Roscoe and J.M. Thomas (1967) The identification and some physico-chemical consequences of non-basal edge and screw dislocations in graphite. *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, 297, 397–407.

[12] J.M. Thomas and C. Roscoe (1968) Nonbasal dislocations in graphite. In P.L. Walker (Ed.), *Chemistry and Physics of Carbon*, Vol. 3, Marcel Dekker, New York.

[13] Y. Kobayashi K. Fukui, T. Enoki, K. Kusakabe and Y. Kaburagi (2005) Observation of zigzag and armchair edges of graphite using scanning tunneling microscopy and spectroscopy. *Physical Review B,* 71, 1934061–1934064.

[14] J.H. Warner, F. Schaffel, M.H. Rummeli and B. Buchner (2009) Examining the edges of multi-layer graphene sheets. *Chemistry of Materials*, 21, 2418-2421.

[15] J.M. Thomas and E.E.G. Hughes (1964) Localized oxidation rates on graphite surfaces by optical microscopy. *Carbon*, 1, 209–214.

[16] M. Wissler (2006) Graphite and carbon powders for electrochemical applications. *Journal of Power Sources*, 156, 142–150.

[17] F.J. Luque, J.D. Pasteris, B. Wopenka, M. Rodas and J.F. Barranechea (1998) Natural fluid-deposited graphite: Mineralogical characteristics and mechanisms of formation. *American Journal of Science*, 298, 471–498.

[18] J. Kim and B. Kim (2007) Chemical and low-expansion treatments for purifying natural graphite powder. *Physicochemical Problems of Mineral Processing*, 41, 37–49.

[19] X.J. Lu and E. Forssberg (2002) Preparation of high-purity and low-sulphur graphite from Woxna fine graphite concentrate by alkali roasting. *Minerals Engineering*, 15, 755–757.

[20] S. Ragan and H. Marsh (1983) Review: Science and technology of graphite manufacture. *Journal of Materials Science*, 18, 3161–3176.

[21] P.L. Walker (1962) Carbon – an old but new material. *American Scientist*, 50, 259–293.

[22] H.O. Pierson (1993) *Handbook of Carbon, Graphite, Diamond and Fullerenes. Properties, Processing and Applications*. Noyes Publications, New Jersey, US.

[23] A. Oberlin (1989) High-resolution TEM studies of carbonization and graphitization. In P.L. Walker (Ed.), *Chemistry and Physics of Carbon* Vol. 22, Marcel Dekker, New York.

[24] F.G. Emmerich (1995) Evolution with heat treatment of crystallinity in carbons. *Carbon*, 33, 1709–1715.

[25] N.V. Russell, J.R. Gibbins and J. Williamson (1999) Structural ordering in high temperature coal chars and the effect on reactivity. *Fuel*, 78, 803–807.

[26] B. Feng, S.K. Bhatia and J.C. Barry (2002) Structural ordering of coal char during heat treatment and its impact on reactivity. *Carbon*, 40, 481–496.

[27] A. Oya and S. Otani (1979) Catalytic graphitization of carbons by various metals. *Carbon*, 17, 131–137.

[28] A. Velichko, C. Holzapfel and F. Mucklich (2007) 3D characterization of graphite morphologies in cast iron. *Advanced Engineering Materials*, 9, 39–45.

[29] N. Cunningham, M. Lefevre, J.-P. Dodelet, Y. Thomas and S. Pelletier (2005) Structural and mechanical characterization of as-compacted powder mixtures of graphite and phenolic resin. *Carbon*, 43, 3054–3066.

[30] Z. Hongsheng, L. Tongxiang, Z. Jie, L. Ziqiang and T. Chunhe (2006) Research on graphite powders used for HTR-PM fuel elements. *Rare Metals*, 25, 347–350.

[31] Z. Klusek, P.K. Datta and W. Kozlowski (2003) Nanoscale studies of the oxidation and hydrogenation of graphite surface. *Corrosion Science*, 45, 1383–1393.

[32] W.H. Bragg and W.L. Bragg (1913) The structure of the diamond. *Nature*, 91, 557.

[33] P. Debije and P. Scherrer (1916) Interferenz an regellos orientierten Teilchen im Röntgenlicht I. *Physikalische Zeit*schrift, 17, 277–283.

[34] D.R. Lide (1994) *CRC Handbook of Chemistry and Physics*. CRC Press, US.

[35] P. Scherrer (1918) Bestimmung der Größe und der inneren Struktur von Kolloidteilchen mittels Röntgenstrahlen. *Göttinger Nachrichten*, 2, 1.

[36] H.P. Klug and L.E. Alexander (1954) *X-Ray Diffraction Procedures for Polycrystalline Material*. Wiley, New York.

[37] B.E. Warren (1941) X-ray diffraction in random layer lattices. *The Physical Review*, 59, 693–698.

[38] H. Fujimoto and M. Shiraishi (2001) Characterization of unordered carbon using Warren-Bodenstein's equation. *Carbon*, 39, 1753–1761.

[39] L. Lu, V. Sahajwalla, C. Kong and D. Harris (2001) Quantitative X-ray diffraction analysis and its application to various coals. *Carbon*, 39, 1821–1833.

[40] H. Shi, J. Barker, M.Y. Saidi, R. Koksbang and L. Morris (1997) Graphite structure and lithium intercalation. *Journal of Power Sources*, 68, 291–295.

[41] H. Dittrich and M. Wohlfahrt-Mehrens (2001) Stacking fault analysis in layered materials. *International Journal of Inorganic Materials*, 3, 1137–1142.

[42] H.A. Willhelm, B. Croset and G. Medjahdi (2007) Proportion and dispersion of rhombohedral sequences in the hexagonal structure of graphite powders. *Carbon*, 45, 2356–2364.

[43] H. Shi, J. Barker, M.Y. Saidi and R. Koksbang (1996) Structure and lithium intercalation properties of synthetic and natural graphite. *Journal of the Electrochemical Society*, 143, 3466–3472.

[44] S.R. Sails, D.J. Gardiner, M. Bowden, J. Savage and D. Rodway (1996) Monitoring the quality of diamond films using Raman spectra excited at 514.5 nm and 633 nm. *Diamond and Related Materials*, 5, 589–591.

[45] Y. Kawashima and G. Katagari (1995) Fundamentals, overtones, and combinations in the Raman spectrum of graphite. *Physical Review B*, 52, 10053–10059.

[46] Y. Wang, D.C. Alsmeyer and R.L. McCreery (1990) Raman spectroscopy of carbon materials: Structural basis of observed spectra. *Chemistry of Materials*, 2, 557–563.

[47] F. Tuinstra and J.L. Koenig (1970) Raman Spectrum of Graphite. *Journal of Chemical Physics*, 53, 1126–1130.

[48] L. Nikiel and P.W. Jagodzinski (1993) Raman spectroscopic characterization of graphites:a re-evaluation of spectra/structure correlation. *Carbon*, 31, 1313–1317.

[49] L. Nikiel and P.W. Jagodzinski (1993) Raman spectroscopic characterization of the oxidation of nuclear-grade graphites. *Applied Spectroscopy*, 47, 2087–2092.

[50] Y. Maniwa, M. Sato, K. Kume, M.E. Kozlov and M. Tokumoto (1996) Comparative NMR study of new carbon forms. *Carbon*, 34, 1287–1291.

[51] J.C.C. Freitas, F.G. Emmerich, G.R.C. Cernicchiaro, L.C. Sampaio and T.J. Bonagamba (2001) Magnetic susceptibility effects on 13C MAS NMR spectra of carbon materials and graphite. *Solid State Nuclear Magnetic Resonance*, 20, 61–73.

[52] J.D. Clark, C.S. Ghanthan and P.J. Robinson (1979) Investigation of pore structure by a non-steady-state gas diffusion technique. *Journal of Materials Science*, 14, 2937–2940.

[53] S. Brunauer, P. H. Emmett and E. Teller (1938) Adsorption of Gases in Multimolecular Layers *Journal of American Chemical Society*, **60**, 309–319.

[54] J.C. Groen, L.A.A. Peffer and J. Pérez-Ramírez (2003) Pore size determination in modified micro-and mesoporous materials. Pitfalls and limitations in gas adsorption data analysis. *Microporous and Mesoporous Materials*, 60, 1–17.

[55] X. Py, A. Guillot and B. Cagnon (2004) Nanomorphology of activated carbon porosity: geometrical models confronted to experimental facts. *Carbon*, 42, 1743–1754.

[56] C. Lastoskie, K.E. Gubbins and N. Quirke (1993) Pore size heterogeneity and the carbon slit pore: A density functional theory model. *Langmuir*, 9, 2693-2702.

[57] S.K. Bhatia (1998) Determination of pore size distributions by regularization and finite element collocation. *Chemical Engineering Science*, 53, 3239–3249.

[58] L. Babout, P.M. Mummery, T.J. Marrow, A. Tzelepi and P.J. Withers (2005) The effect of thermal oxidation on polycrystalline graphite studied by X-ray tomography. *Carbon*, 43, 765–774.

[59] L. Babout, B.J. Marsden, P.M. Mummery and T.J Marrow (2008) Three-dimensional characterization and thermal property modelling of thermally oxidized nuclear graphite. *Acta Materialia*, 56, 4242–4254.

[60] L.R. Radovic and B. Bockrath (2005) On the chemical nature of graphene edges: Origin of stability and potential for magnetism in crabon materials. *Journal of the American Chemical Society*, 127, 5917–5927.

[61] H.P. Boehm (2002) Surface oxides on carbon and their analysis: a critical assessment. *Carbo*n, 40, 145–149.

[62] M. Barber, E.L. Evans and J.M. Thomas (1973) Oxygen chemisorption on the basal faces of graphite: An XPS study. *Chemical Physics Letters*, 18, 423–425.

[63] A. Contescu, C. Contescu, K. Putyera and J.A. Schwarz (1997) Surface acidity of carbons characterized by their continuous pK distribution and Boehm titration. *Carbon*, 35, 83–94.

[64] A. Contescu, M. Vass, C. Contescu, K. Putyera and J.A. Schwarz (1998) Acid buffering capacity of basic carbons revealed by their continuous pK distribution. *Carbon*, 36, 247–258.

[65] M. Domingo-Garcia, F.J. Lopez-Garzon and M.J. Perez-Mendoza (2002) On the characterization of chemical surface groups of carbon materials. *Journal of Colloid and Interface Science*, 248, 116–122.

[66] P.J.F. Harris (2005) New perspectives on the structure of graphitic carbons. *Critical Reviews in Solid State and Materials Sciences*, 30, 235–253.

[67] D.S. Knight and W.B. White (1989) Characterization of diamond films by Raman spectroscopy. *Journal of Materials Research*, 4, 385–393.

[68] N.J. Welham, V. Berbenni and P.G. Chapman (2003) Effect of extended ball milling on graphite. *Journal of Alloys and Compounds*, 349, 255–263.

[69] N.J. Welham and J.S. Williams (1998) Extended milling of graphite and activated carbon. *Carbon*, 36, 1309–1315.

[70] M. Endo, C. Kim, T. Karaki, T. Tamaki, Y. Nishimura, M.J. Matthews, S.D.M. Brown and M.S. Dresselhaus (1998) Structural analysis of the B-doped mesophase pitch-based graphite fibers by Raman spectroscopy. *Physical Review B*, 58, 8991–8996.

[71] V.I. Merkulov, J.S. Lannin, C.H. Munro, S.A. Asher, V.S. Veerasamy and W.I. Milne (1997) UV studies of tetrahedral bonding in diamondlike amorphous carbon. *Physical Review Letters*, 78, 4869–4872.

[72] C.Z. Wang and K.M. Ho (1993) Structure, dynamics and electronic properties of diamondlike amorphous carbon. *Physical Review Letters*, 71, 1184–1188.

[73] J. Schwan, V. Batori, S. Ulrich, H. Ehrhardt and S.R.P. Silva (1998) Nitrogen doping of amorphous carbon thin films. *Journal of Applied Physics*, 84, 2071–2081.

[74] A.C. Ferrari and J. Robertson (2001) Origin of the 1150 cm^{-1} Raman mode in nanocrystalline diamond. *Physical Review B*, 63, 1214051–1214054.

[75] P.K. Bachmann (1996) *Ullman's Encyclopaedia of Industrial Chemistry,* Vol. A26. Wiley, New York.

[76] A.C. Ferrari and J. Robertson (2000) Interpretation of Raman spectra of disordered and amorphous carbon. *Physical Review B*, 61, 14095–14107.

[77] T.D. Burchell (1999) *Carbon Materials for Advanced Technologies*. Pergamon, Amsterdam.

[78] R.E. Franklin (1951) Crystallite growth in graphitizing and non-graphitizing carbons. *Proceedings of the Royal Society of London*, 209, 196–218.

[79] L.L. Ban, D. Crawford and H. Marsh (1975) Lattice-resolution electron microscopy in structural studies of non-graphitizing carbons from polyvinylidene chloride (PVDC). *Journal of Applied Crystallography*, 8, 415–420.

[80] D. Crawford and D.J. Johnson (1971) High-resolution electron microscopy of high-modulus carbon fibres. *Journal of Microscopy*, 94, 51–62.

[81] A. Kumar, R.F. Lobo and N.J. Wagner (2005) Porous amorphous carbon models from periodic Gaussian chains of amorphous polymers. *Carbon*, 43, 3099–3111.

[82] Renewable Energy Policy Network (2009) Renewables 2010 Global Status Report. Review Report. Available at: http://www.ren21.net/REN21Activities/Publications/Global StatusReport /tabid/5434/Default.aspx.

[83] British Petroleum (2010) BP Statistical Review of World Energy. Review report. Available at: http://www.bp.com/productlanding.do?categoryId=6929&contentId=704462.

[84] P.L. Walker, Jr., F. Rusinko, Jr. and L.G. Austin (1959) Gas reactions of carbon. *Advances in Catalysis and Related Subjects*, 11, 133–221.

[85] E.A. Gulbransen and K.F. Andrew (1952) Reactions of artificial graphite: Surface oxide formation and surface roughness studies in relation to oxidation of artificial graphite at temperatures of 25 °C and between 425 to 575 °C. *Industrial and Engineering Chemistry*, 44, 1039–1044.

[86] J.M. Smith, H.C. van Ness and M.M. Abbott (2001) *Chemical Engineering Thermodynamics.* McGraw-Hill, New York.

[87] H.P. Boehm (1973) Carbon from carbon monoxide disproportionation on nickel and iron catalysts: Morphological studies and possible growth mechanisms. *Carbon*, 11, 583–590.

[88] A.N. Hayhurst and M.S. Parmar (1998) Does solid carbon burn in oxygen to give the gaseous intermediate CO or produce CO2 directly? Some experiments in a hot bed of sand fluidized by air. *Chemical Engineering Science*, 53, 427–438.

[89] I.M. Bews, A.N. Hayhurst, S.M. Richardson and S.G. Taylor (2001) The order, Arrhenius parameters, and mechanism of the reaction between gaseous oxygen and solid carbon. *Combustion and Flame*, 124, 231–245.

[90] F. Scala (2009) A new technique for the measurement of the product CO/CO_2 ratio at the surface of char particles burning in a fluidized bed. *Proceedings of the Combustion Institute*, 32, 2021–2027.

[91] R. Phillips, F.J. Vastola and P.L. Walker Jr (1970) Factors affecting the product ratio of the carbon-oxygen reaction. II. Reaction temperature. *Carbon*, 8, 205–210.

[92] E.T. Turkdogan, V. Koump, J.V. Vinters and T.F. Perzak (1968) Rate of oxidation of graphite in carbon dioxide. *Carbon*, 6, 467–484.

[93] E.T. Turkdogan and J.V. Vinters (1970) Effect of carbon monoxide on the rate of oxidation of charcoal, graphite and coke in carbon dioxide. *Carbon*, 8, 39–53.

[94] G. Blyholder and H. Eyring (1957) Kinetics of graphite oxidation. Journal of Physical Chemistry, 61, 682–688.

[95] R.H. Hurt and B.S. Haynes (2005) On the origin of power-law kinetics in carbon oxidation. *Proceedings of the Combustion Institute*, 30, 2161–2168.

[96] R. Phillips, F.J. Vastola and P.L. Walker Jr (1969) The effect of oxygen pressure and carbon burn-off on the product ratio of the carbon-oxygen reaction. *Carbon*, 7, 479–485.

[97] J.J. Murphy and C.R. Shaddix (2010) Effect of reactivity loss on apparent reaction order of burning char particles. *Combustion and Flame*, 157, 535–539.

[98] J. Hong, W.C. Hecker and T.H. Fletcher (2000) Modelling high-pressure char oxidation using Langmuir kinetics with an effectiveness factor. *Proceedings of the Combustion Institute*, 28, 2215–2223.

[99] D. Zeng (2005) Effect of pressure on coal pyrolysis at high heating rates and char combustion. PhD Thesis, Brigham Young University, US.

[100]E.L. Fuller and J.M. Okoh (1997) Kinetics and mechanisms of reaction of air with nuclear-grade graphites: IG-110. *Journal of Nuclear Materials*, 240, 241–250.

[101] C. Di Blasi, F. Buonanno and C. Branca (1999) Reactivities of some biomass chars in air. *Carbon*, 37, 1227–1238.

[102] I.W. Smith (1982) The combustion rates of coal chars: A review. *Proceedings of the 19th Symposium on Combustion*, 1045–1065.

[103] W.A. Propp (1998) *Graphite Oxidation: Kinetics/Thermodynamics*. Idaho National Engineering and Environmental Laboratory,1–21.

[104] H.S. Fogler (1999) *Elements of Chemical Reaction Engineering*. Prentice Hall, New Jersey.

[105] D.F. Fairbanks and C.R. Wilke (1950) Diffusion coefficients in multicomponent gas mixtures. *Industrial and Engineering Chemistry*, 471.

[106] H.F. Stoeckli (1990) Microporous carbons and their characterization: The present state of the art. *Carbon*, 28, 1–6.

[107] T. Kyotani (2000) Control of pore structure in carbon. *Carbo*n, 38, 269–286.

[108] S. Kulasekaran, T.M. Linjewile, P.K. Agarwal and M.J. Biggs (1998) Combustion of a porous char particles in an incipiently fluidized bed. *Fuel*, 77, 1549–1560.

[109] A.N. Hayhurst (2000) The mass transfer coefficient for oxygen reacting with a carbon particle in a fluidized or packed bed. *Combustion and Flame*, 121, 679–688.

[110] R. Hurt, J.K. Sun and M. Lunden (1998) A kinetic model of carbon burnout in pulverized coal combustion. *Combustion and Flame*, 113, 181–197.

[111] A.K. Sadhukhan, P. Gupta and R.K. Saha (2008) Analysis of the dynamics of coal char combustion with ignition and extinction phenomena: Shrinking core model. *International Journal of Chemical Kinetics*, 40, 569–582.

[112] J. Lachaud, N. Bertrand, G.L. Vignoles, G. Bourget, F. Rebillat and P. Weisbecker (2007) A theoretical/experimental approach to the intrinsic oxidation reactivities of C/C composites and of their components. *Carbon*, 45, 2768–2776.

[113] F. Gelbard (2009) Graphite oxidation modeling for application in Melcor. New Mexico, US, Sandia National Laboratories Report, 1–43.

[114] B. Duval, J.M. Guet, J.R. Richard and J.N. Rouzaud (1988) Coke properties and their microtexture. Part III: First results about relationship between microtexture and reactivity of some cokes. *Fuel Processing Technology*, 20, 163–175.

[115] J.P. Olivier (1998) Improving the models used for calculating the size distribution of micropore volume of activated carbons from adsorption data. *Carbon*, 36, 1469–1472.

[116] P.A. Gauden, A.P. Terzyk and P. Kowalczyk (2006) Some remarks on the calculation of the pore size distribution function of activated carbons. *Journal of Colloid and Interface Science*, 300, 453–474.

[117] N. Setoyama, T. Suzuki and K. Kaneko (1998) Simulation study on the relationship between a high resolution alpha s-plot and the pore size distribution for activated carbon. *Carbon*, 36, 1459–1467.

[118] S.K. Bhatia and D.D. Perlmutter (1980) A random pore model for fluid-solid reactions. I. Isothermal, kinetic control. *AIChE Journal*, 26, 379–385.

[119] J.-L. Su and D.D. Perlmutter (1985) Effect of pore structure on char oxidation kinetics. *AIChE Journal*, 31, 973–981.

[120] J.-L. Su and D.D. Perlmutter (1984) Evolution of pore volume distribution during gasification. *AIChE Journal*, 30, 967–973.

[121] M. Sahimi, G.R. Gavalas and T.T. Tsotsis (1990) Statistical and continuum models of fluid-solid reactions in porous media. *Chemical Engineering Science*, 45, 1443–1502.

[122] S.K. Bhatia and B.J. Vartak (1996) Reaction of microporous solids: The discrete random pore model. *Carbon*, 34, 1383–1391.

[123] S.K. Bhatia (1998) Reactivity of chars and carbons: New insights through molecular modelling. *AIChE Journal*, 44, 2478–2493.

[124] J. Srinivasalu Gupta and S.K. Bhatia (2000) A modified discrete random pore model allowing for different initial surface reactivity. *Carbon*, 38, 47–58.

[125] F.Y. Wang and S.K. Bhatia (2001) A generalised dynamic model for char particle gasification with sturcture evolution and peripheral fragmentation. *Chemical Engineering Science*, 56, 3683–3697.

[126] J.-L. Su and D.D. Perlmutter (1985) Porosity effects on catalytic char oxidation. Part I. A catalyst deposition model. *AIChE Journal*, 31, 957–964.

[127] Y. Zhang, M. Ashizawa, S. Kajitani and K. Miura (2008) Proposal of a semi-empirical kinetic model to reconcile with gasification reactivity profiles of biomass char. *Fuel*, 87, 475–481.

[128] T.X. Nguyen and S.K. Bhatia (2006) Characterization of heat-treated porous carbons and argon adsorption. *Carbon*, 44, 646–652.

[129] J.M. Thomas (1969) Topographical studies of oxidized graphite surfaces: A summary of the present position. *Carbon*, 7, 350–364.

[130] C.W. Zielke and E. Gorin (1957) Kinetics of carbon gasification. *Industrial and Engineering Chemistry*, 49, 396–403.

[131] A.D. Kirshenbaum (1977) Effect of different carbons on ignition temperature and activation energy of black powder. *Thermochimica Acta*, 18, 113–123.

[132] N.R. Laine, F.J. Vastola and P.L. Walker, Jr (1963) Importance of active surface area in the carbon-oxygen reaction. *Journal of Physical Chemistry*, 67, 2030–2034.

[133] N.R. Laine, F.J. Vastola and P.L. Walker, Jr (1963) The role of the surface complex in the carbon-oxygen reaction. *Proceedings of the 5th Carbon Conference*, 2, 211–217.

[134] S.B. Tong, P. Pareja and M.H. Back (1982) Correlation of the reactivity, the active surface area and the total surface area of thin films of pyrolytic carbon. *Carbon*, 20, 191–194.

[135] L.R. Radovic, P.L. Walker Jr and R.G. Jenkins (1983) Importance of carbon active sites in the gasification of coal chars. *Fuel*, 62, 849–856.

[136] J.-L. Su and D.D. Perlmutter (1985) Effect of chemisorbed oxygen on char reactivity. *AIChE Journal*, 31, 1725–1727.

[137] A. Arenillas, F. Rubiera, C. Pevida, C.O. Ania and J.J. Pis (2004) Relationship between structure and reactivity of carbonaceous materials. *Journal of Thermal Analysis and Calorimetry*, 76, 593–602.

[138] F.J. Vastola, P.J. Hart and P.L. Walker, Jr (1964) A study of carbon-oxygen surface complexes using O-18 as a tracer. *Carbon*, 2, 65–71.

[139] P.L. Walker, Jr., F.J. Vastola and P.J. Hart (1967) Oxygen-18 tracer studies of the carbon-oxygen reaction. *Fundamentals of Gas-Surface Interactions*, 307–316.

[140] R.O. Lussow, F.J. Vastola and P.L. Walker, Jr (1967) Kinetics of oxygen interaction with graphon between 450 and 675 degrees C. *Carbon*, 5, 591–602.

[141] R.C. Bansal, F.J. Vastola and P.L. Walker, Jr (1970) Studies on ultra-clean carbon surfaces. IV. Decomposition of carbon-oxygen surface complexes. *Carbon*, 8, 443–448.

[142] R. Phillips, F.J. Vastola and P.L. Walker, Jr (1970) The thermal decomposition of surface oxides formed on graphon. *Carbon*, 8, 197–203.

[143] P.J. Hall and J.M. Calo (1989) Secondary interactions upon thermal desportion of surface oxides from coal chars. *Energy & Fuels*, 3, 370–376.

[144] A.A. Lizzio, A. Piotrowski and L.R. Radovic (1988) Effect of oxygen chemisorption on char gasification reactivity profiles obtained by thermogravimetric analysis. *Fuel*, 67, 1691–1695.

[145] B. Feng and S.K. Bhatia (2002) On the validity of thermogravimetric determination of carbon gasification kinetics. *Chemical Engineering Science*, 57, 2907–2920.

[146] J.G. Brown, J. Dollimore, C.M Freedman and B.H. Harrison (1970) The use of partial-pressure mass spectrometry in the thermal analysis study of carbons and graphite. *Thermochimica Acta*, 1, 499–508.

[147] S.S. Barton, B.H. Harrison and J. Dollimore (1972) Surface studies on graphite: Desorption of surface oxide. *Journal of Physical Chemistry*, 82, 825–834.

[148] P.L. Walker Jr, R.L. Taylor and J.M. Ranish (1991) An update on the carbon-oxygen reaction. *Carbon*, 29, 411–421.

[149] A.A. Lizzio, H. Jiang and L.R. Radovic (1990) On the kinetics of carbon (char) gasification: Reconciling models with experiments. *Carbon*, 28, 7–19.

[150] L.R. Radovic, H. Jiang and A.A. Lizzio (1991) A transient kinetics study of char gasification in carbon dioxide and oxygen. *Energy & Fuels*, 5, 68–74.

[151] R.N. Smith, D.A. Young and R.A. Smith (1966) Infra-red study of carbon-oxygen surface complexes. *Transactions of the Faraday Society*, 62, 2280–2286.

[152] M. Starsinic, R.L. Taylor, P.L. Walker, Jr. and P.C. Painter (1983) FTIR studies of saran chars. *Carbon*, 21, 69–74.

[153] B. Marchon, W.T. Tysoe, J. Carrazza, H. Heinemann and G.A. Somorjai (1988) Reactive and kinetic properties of carbon monoxide and carbon dioxide on a graphite surface. *Journal of Physical Chemistry*, 92, 5744–5749.

[154] B. Marchon, J. Carrazza, H. Heinemann and G.A. Somorjai (1988) TPD and XPS studies of O_2, CO_2 and H_2O adsorption on clean polycrystalline graphite. *Carbon*, 26, 507–514.

[155] T.C. Brown and B.S. Haynes (1992) Interaction of CO with carbon and carbon surface oxides. *Energy & Fuels*, 6, 154–159.

[156] A. Sibraa, T. Newbury and B.S. Haynes (2000) The reactions of hydrogen and carbon monoxide with surface-bound oxides on carbon. *Combustion and Flame*, 120, 515–525.

[157] B. Henschke, H. Schubert, J. Blöcker, F. Atamny and R. Schlögl (1994) Mechanistic aspects of the reaction between carbon and oxygen. *Thermochimica Acta*, 234, 53–83.

[158] Q-L. Zhuang, T. Kyotani and A. Tomita (1994) DRIFT and TK/TPD analyses of surface oxygen complexes formed during carbon gasification. *Energy & Fuels*, 8, 714–718.

[159] Q-L. Zhuang, T. Kyotani and A. Tomita (1994) The change of TPD pattern of O_2-gasified carbon upon air exposure. *Carbon*, 32, 539–540.

[160] Q-L. Zhuang, T. Kyotani and A. Tomita (1995) Dynamics of surface oxygen complexes during carbon gasification with oxygen. *Energy & Fuels*, 6, 494–497.

[161] J.L. Figueiredo, M.F.R. Pereira, M.M.A. Freitas and J.J.M. Orfao (1999) Modification of surface chemistry of activated carbons. *Carbon*, 37, 1379–1389.

[162] G.S. Szymanski, Z. Karpinski, S. Biniak and A. Swiatkowski (2002) The effect of the gradual thermal decomposition of oxygen species on the chemical and catalytic properties of oxidized activated carbon. *Carbon*, 20, 2627–2639.

[163] J-H. Zhou, Z-J. Sui, J. Zhu, P. Li, D. Chen, Y-C. Dai and W-K. Yuan (2007) Characterization of surface oxygen complexes on carbon nanofibres by TPD, XPS and FT-IR. *Carbon*, 45, 785–796.

[164] Z. Pan and R.T. Yang (1992) Strongly bonded oxygen in graphite: Detection by high-temperature TPD and characterization. *Industrial and Engineering Chemistry Research*, 31, 2675–2680.

[165] F. Kapteijn, R. Meijer and J.A. Moulijn (1992) Transient kinetic techniques for detailed insight in gas-solid reactions. *Energy & Fuels*, 6, 494–497.

[166] F. Kapteijn, R. Meijer, J.A. Moulijn and D. Cazorla-Amorós (1994) On why do different carbons show different gasification rates? Transient isotopic CO_2 gasification study. *Carbon*, 32, 1223–1231.

[167] S.G. Chen, R.T. Yang, F. Kapteijn and J.A. Moulijn (1993) A new surface oxygen complex on carbon: Toward a unified mechanism for carbon gasification reactions. *Industrial and Engineering Chemistry Research*, 32, 2835–2840.

[168] J.A. Moulijn and F. Kapteijn (1995) Towards a unified theory of reactions of carbon with oxygen-containing molecules. *Carbon*, 33, 1155–1165.

[169] S.G. Chen and R.T. Yang (1997) Unified mechanism of alkali and alkaline earth catalyzed gasification reactions of carbon by CO_2 and H_2O. *Energy & Fuels*, 11, 421–427.

[170] N. Chen and R.T. Yang (1998) *Ab initio* molecular orbital calculation on graphite: Selection of molecular system and model chemistry. *Carbon*, 36, 1061–1070.

[171] R. Backreedy, J.M. Jones, M. Pourkashanian and A. Williams (2001) A study of the reaction of oxygen with graphite: Model chemistry. *Faraday Discussions*, 119, 385–394.

[172] A. Montoya, T-T.T. Truong, F. Mondragón and T.N. Truong (2001) CO desorption from oxygen species on carbonaceous surface. 1. Effects of the local structure of the active site and surface coverage. *Journal of Physical Chemistry A*, 105, 6757–6764.

[173] Z.H. Zhu, J. Finnerty, G.Q. Lu and R.T. Yang (2002) A comparative study of carbon gasification with O_2 and CO_2 by density functional theory calculations. *Energy & Fuels*, 16, 1359–1368.

[174] J.F. Espinal, A. Montoya, F. Mondragón and T.N. Truong (2004) A DFT study of interaction of carbon monoxide with carbonaceous materials. *Journal of Physical Chemistry B*, 108, 1003–1008.

[175] K. Sendt and B.S. Haynes (2005) Density functional study of the reaction of carbon surface oxides: The behaviour of ketones. *Journal of Physical Chemistry* A, 109, 3438–3447.

[176] A. Allouche and Y. Ferro (2006) Dissociative adsorption of small molecules at vacancies on the graphite (0001) surface. *Carbon*, 44, 3320–3327.

[177] J.M. Jones and D.H. Jones (2007) Modelling the competition between annealing and oxidation in the carbon-oxygen reaction. *Carbon*, 45, 668–689.

[178] Z.H. Zhu, J. Finnerty, G.Q. Lu and R.T. Yang (2003) Electronic structure methods applied to gas-carbon reactions. *Carbon*, 41, 635–658.

[179] N. Chen and R.T. Yang (1998) *Ab initio* molecular orbital study of the unified mechanism pathways for gas-carbon reactions. *Journal of Physical Chemistry A*, 102, 6348–6356.

[180] A. Montoya, T.N. Truong and A.F. Sarofim (2000) Spin contamination in Hartree-Fock and density functional theory wavefunctions in modelling of adsorption on graphite. *Journal of Physical Chemistry A*, 102, 6108–6110.

[181] A. Montoya, F. Mondragón and T.N. Truong (2002) Formation of CO precursors during char gasification with O_2, CO_2 and H_2O. *Fuel Processing Technology*, 77, 125–130.

[182] A. Montoya, F. Mondragón and T.N. Truong (2002) First-principles kinetics of CO desorption from oxygen species on carbonaceous surface. *Journal of Physical Chemistry A*, 106, 4236–4239.

[183] T.J. Frankcombe and S.C. Smith (2004) On the microscopic mechanism of carbon gasification: A theoretical study. *Carbon*, 42, 2921–2928.

[184] Y-J. Xu and J-Q. Li (2005) The interaction of molecular oxygen with active sites of graphite: A theoretical study. *Chemical Physics Letters*, 400, 406–412.

[185] L.R. Radovic (2005) The mechanism of CO_2 chemisorption on zigzag carbon active sites: A computational chemistry study. *Carbon*, 43, 907–915.

[186] K. Sendt and B.S. Haynes (2005) Density functional study of the chemisorption of O_2 on the armchair surface of graphite. *Proceedings of the Combustion Institute*, 30, 2141–2149.

[187] K. Sendt and B.S. Haynes (2005) Density functional study of the chemisorption of O_2 on the zig-zag surface of graphite. *Combustion and Flame*, 143, 629–643.

[188] K. Sendt and B.S. Haynes (2007) Density functional study of the chemisorption of O_2 across two rings of the armchair surface of graphite. *Journal of Physical Chemistry C*, 111, 5465–5473.

[189] E.A. Gulbransen (1952) Reactions of artificial graphite: Mechanism of the oxidation of graphite at temperatures of 425 to 575 °C. *Industrial and Engineering Chemistry*, 44, 1045–1047.

[190] E.A. Gulbransen and K.F. Andrew (1952) Reactions of artificial graphite: Kinetics of oxidation of artificial graphite at temperatures of 425 to 575°C and pressures of 0.15 to 9.8 cm. of mercury of oxygen. *Industrial and Engineering Chemistry*, 44, 1034–1038.

[191] G. Blyholder and H. Eyring (1959) Kinetics of graphite oxidation II. *Journal of Physical Chemistry*, 63, 1004–1008.

[192] E.A. Gulbransen, K.F. Andrew and F.A. Brassart (1963) The oxidation of graphite at temperatures of 600° to 1500°C and at pressures of 2 to 76 torr of oxygen. *Journal of the Electrochemical Society*, 110, 476–483.

[193] J.N. Ong, Jr (1964) On the kinetics of oxidation of graphite. Carbon, 2, 281–297.

[194] E.L. Evans, R.J.M. Griffiths and J.M. Thomas (1971) Kinetics of single-layer graphite oxidation: Evaluation by electron microscopy. *Science*, 171, 174–175.

[195] H. Chang and A.J. Bard (1991) Scanning tunneling microscopy studies of carbon-oxygen reactions on highly oriented pyrolytic graphite. *Journal of the American Chemical Society*, 113, 5588–5596.

[196] D. Tandon, E.J. Hippo, H. Marsh and E. Sebok (1997) Surface topography of oxidized HOPG by scanning tunelling microscopy. *Carbon*, 35, 35–44.

[197] J.I. Paredes, A. Martinez-Alonso and J.M.D. Tascon (2000) Comparative study of the air and oxygen plasma oxidation of highly oriented pyrolytic graphite: A scanning tunneling and atomic force microscopy investigation. *Carbon*, 38, 1183–1197.

[198] N.J. Curson, R.J. Wilson, L.A. Silva, W. Allison and G.A.C Jones (1999) Studying the kinetics of graphite oxidation using a scanning tunnelling

microscope – An undergraduate laboratory experiment. *European Journal of Physics*, 20, 453–460.

[199] Y.J. Zhu, T.A. Hansen, S. Ammermann, J.D. McBride and T.P. Beebe, Jr (2001) Nanometer-size monolayer and multilayer molecule corrals on HOPG: a depth-resolved mechanistic study by STM. *Journal of Physical Chemistry B*, 105, 7632–7638.

[200] F. Stevens, L.D. Kolodny and T.P. Beebe, Jr (1998) Kinetics of graphite oxidation: Monolayer and multilayer etch pits in HOPG studied by STM. *Journal of Physical Chemsitry B*, 102, 10799–10804.

[201] J.R. Hahn, H. Kang, S.M. Lee and Y.H. Lee (1999) Mechanistic study of defect-induced oxidation of graphite. *Journal of Physical Chemsitry B*, 103, 9944–9951.

[202] J.R. Hahn (2005) Kinetic study of graphite oxidation along two lattice directions. *Carbon*, 43, 1506–1511.

[203] S. Ahmed and M.H. Back (1985) The role of the surface complex in the kinetics of the reaction of oxygen with carbon. *Carbon*, 23, 513–524.

[204] O.S. Özgen and B. Rand (1985) Kinetics of oxidation of the graphite phase in alumina/graphite materials. I. Effect of temperature and initial pore structure at a fixed graphite content. *British Ceramic Transactions Journal*, 84, 70–76.

[205] L.E.C. de Torre, J.L. Llanos and E.J. Bottani (1991) Graphite oxidation in air at different temperatures. *Carbon*, 29, 1051–1061.

[206] K. Zaghib, X. Song and K. Kinoshita (2001) Thermal analysis of the oxidation of natural graphite: Isothermal kinetic studies. *Thermochimica Acta*, 371, 57–64.

[207] E.S. Kim, K.W. Lee and H.C. No (2006) Analysis of geometrical effects on graphite oxidation through measurement of internal surface area. *Journal of Nuclear Materials*, 348, 174–180.

[208] L. Xiaowei, R. Jean-Charles and Y. Suyuan (2004) Effect of temperature on graphite oxidation behaviour. *Nuclear Engineering and Design*, 227, 273–280.

[209] R. Moormann and H.-K. Hinssen (2001) Advanced graphite oxidation models. basic studies in the field of high-temperature engineering.

Proceedings of the Second Information Exchange Meeting on Basic Studies in the Field of High-Temperature Engineering, 243–254.

[210] H.-K. Hinssen, K. Kühn, R. Moormann, B. Schlögl, M. Fechter and M. Mitchell (2008) Oxidation experiments and theoretical examinations on graphite materials relevant for the PBMR. *Nuclear Engineering and Design*, 233, 251–260.

[211] X. Yu, L. Brissonneau, C. Bourdeloie and S. Yu (2008) The modelling of graphite oxidation behaviour for HTGR fuel coolant channels under normal operating conditions. *Nuclear Engineering and Design*, 238, 1-9.

[212] H.K. Chelliah, A. Makino, I. Kato, N. Araki and C.K. Law (1996) Modeling of graphite oxidation in a stagnation-point flow field using detailed homogeneous and semiglobal heterogeneous mechanisms with comparisons to experiments. *Combustion and Flame*, 104, 469–480.

[213] E.S. Kim, H.C. No (2006) Experimental study on the oxidation of nuclear graphite and development of an oxidation model. *Journal of Nuclear Materials*, 349, 182–194.

[214] R.H. Hurt and J.M. Calo (2001) Semi-global intrinsic kinetics for char combustion modeling. *Combustion and Flame*, 125, 1138–1149.

[215] R.H. Essenhigh (1981) Chemistry of Coal Utilization. Wiley, New York.

[216] J.M. Ranish, P.L. Walker, Jr (1993) High pressure studies of the carbon-oxygen reaction. *Carbon*, 31, 135–141.

[217] R.J. Sawaya, J.W. Allen, W.C. Hecker, T.H. Fletcher and L.D. Smoot (1999) Kinetics of high pressure char oxidation. *ACS Division of Fuel Chemistry*, 44, 1016–1019.

[218] B.S. Haynes and T.G. Newbury (2000) Oxyreactivity of carbon surface complexes. *Proceedings of the Combustion Institute*, 28, 2197–2203.

[219] B.S. Haynes (2001) A turnover model for carbon reactivity. I. Development. *Combustion and Flame*, 126, 1421–1432.

[220] P.A. Campbell and R.E. Mitchell (2008) The impact of the distribution of surface oxides and their migration on characterization of the heterogeneous carbon-oxygen reaction. *Combustion and Flame*, 1–20.

[221] D.L. Battye and P.J. Ashman (2009) The stoichiometry and kinetics of carbon combustion at low temperature: A surface complex approach. *Proceedings of the Combustion Institute*, 32, 1981–1988.

[222] C. Li and T.C. Brown (2001) Carbon oxidation kinetics from evolved carbon oxide analysis during temperature-programmed oxidation. *Carbon*, 39, 725–732.

[223] S. Cebulak, B. Smieja-Krol, S. Duber, M. Misz and A.W. Morawski (2004) Oxyreactive thermal analysis: A good tool for the investigation of carbon materials. *Journal of Thermal Analysis and Calorimetry*, 77, 201–206.

[224] R. Moormann, H.-K. Hinssen and K. Kühn (2004) Oxidation behaviour of an HTR fuel element matrix graphite in oxygen compared to a standard nuclear graphite. *Nuclear Engineering and Design*, 227, 281–284.

[225] J.A. Turner and K.M. Thomas (1997) The application of simultaneous TG-DTA to the determination of the fate of injected coal in a pilot-scale blast furnace simulation rig. *Thermochimica Acta*, 294, 51–56.

[226] A.K. Bhattacharyya, P. Bondopadhyah and P. Das (2003) Oxidation reaction in graphite – Role of particle characteristics. *Ceramics International*, 29, 967–969.

[227] A.K. Bhattacharyya, P. Bondopadhyah and P. Das (2004) A modification of Ozen's first order diffusion kinetics reaction during carbon oxidation at higher temperatures. *Ceramics International*, 30, 485–487.

[228] W. Guo, H. Xiao and W. Guo (2008) Modelling of TG curves of isothermal oxidation of graphite. *Materials Science and Engineering*, 474, 197–200.

[229] E. Breval, M. Klimkiewicz, D.K. Agrawal and F. Rusinko, Jr (2002) Pinhole formation and weight loss during oxidation of industrial graphite and carbon. *Carbon*, 40, 1017–1027.

[230] B. Meng and W.H. Weinberg (1994) Monte Carlo simulations of temperature programmed desorption spectra. *Journal of Chemical Physics*, 100, 5280–5289.

[231] T. Kyotani, K.-I. Ito, A. Tomita and L.R. Radovic (1996) Monte Carlo simulation of carbon gasification using molecular orbital theory. *AIChE Journal*, 42, 2303–2307.

[232] F. Stevens and T.P. Beebe Jr (1999) Computer modelling of graphite oxidation: Differences between monolayer and multilayer etching. *Computers and Chemistry*, 23, 175–183.

[233] G. Hall, B.J. Marsden and S.L. Fok (2006) The microstructural modelling of nuclear grade graphite. *Journal of Nuclear Materials*, 353, 12–18.

[234] A.K. Galwey (2008) What can we learn about the mechanisms of thermal decompositions of solids from kinetic measurements? *Journal of Thermal Analysis and Calorimetry*, 92, 967–983.

[235] A.K. Galwey and M.E. Brown (2002) Application of the Arrhenius equation to solid state kinetics: Can this be justified? *Thermochimica Acta*, 386, 91–98.

[236] J. Šesták and G. Berggren (1971) Study of the kinetics of the mechanism of solid-state reactions at increasing temperatures. *Thermochimica Acta*, 3, 1–12.

[237] A.K. Galwey and M.E. Brown (2007) An appreciation of the chemical approach of V.V. Boldyrev to the study of the decomposition of solids. *Journal of Thermal Analysis and Calorimetry*, 90, 9–22.

[238] A.K. Galwey (2004) Is the science of thermal analysis kinetics based on solid foundations? A literature appraisal. *Thermochimica Acta*, 413, 139–183.

[239] N. Koga and H. Tanaka (2002) A physico-geometric approach to the kinetics of solid-state reactions as exemplified by the thermal dehydration and decomposition of inorganic solids. *Thermochimica Acta*, 388, 41–61.

[240] N. Koga (1997) Physico-geometric kinetics of solid-state reactions by thermal analyses. *Journal of Thermal Analysis and Calorimetry*, 49, 45–56.

[241] M. Avrami (1939) Kinetics of phase change. I. General theory. Journal of Chemical Physics, 7, 1103.

[242] M. Avrami (1940) Kinetics of phase change. II. Transformation-time relations for random distribution of nuclei. *Journal of Chemical Physics*, 8, 212.

[243] M. Avrami (1941) Granulation, phase change, and microstructure kinetics of phase change. III. *Journal of Chemical Physics*, 9, 177.

[244] B.V. Erofeev (1946) A generalized chemical kinetics equation and its application to reactions involving the participation of solid substances. *Dokl. Akad. Nauk SSSR*, 52, 511.

[245] E.G. Prout and F.C. Tompkins (1944) The thermal decomposition of potassium permanganate. *Transactions of the Faraday Society*, 40, 488–498.

[246] W. Jander (1927) Reactions in the solid state at high temperatures. *Z. Anorg. Allgem. Chem*., 163, 1.

[247] A.M. Ginstling and B.I. Brounshtein (1950) On diffusion kinetics in chemical reactions taking place in spherical powder grains. *Zhur. Priklad. Khim*., 23, 1249.

[248] A. Khawam and D.R. Flanagan (2006) Solid-state kinetic models: Basics and mathematical fundamentals. *Journal of Physical Chemistry* B, 110, 17315–17328.

[249] A.K. Galwey and M.E. Brown (1999) Thermal Decomposition of Ionic Solids. Elsevier, Amsterdam.

[250] M.E. Brown (1997) The Prout-Tompkins rate equation in solid-state kinetics. *Thermochimica Acta*, 300, 93–106.

[251] L.A. Perez-Maqueda, J.M. Criado and P.E. Sanchez-Jimenez (2006) Combined kinetic analysis of solid-state reactions: A powerful tool for the simultaneous determination of kinetic parameters and the kinetic model without previous assumptions on the reaction mechanism. *Journal of Physical Chemistry A*, 110, 12456–12462.

[252] J.M. Criado and J. Morales (1977) Thermal decomposition reactions of solids controlled by diffusion and phase-boundary processes: Possible misinterpretation of the mechanism from thermogravimetric data. *Thermochimica Acta*, 19, 305–317.

[253] J.M. Criado, M.Gonzalez, A.Ortega and C. Real (1984) Some considerations regarding the determination of the activation energy of solid-state reactions from a series of isothermal data. *Journal of Thermal Analysis and Calorimetry*, 29, 243–250.

[254] T. Ozawa (1984) Nonisothermal kinetics of crystal growth from preexisting nuclei. *Bulletin of the Chemical Society of Japan*, 57, 639–643.

[255] N. Koga (1995) Kinetic analysis of thermoanalytical data by extrapolation to infinite temperature. *Thermochimica Acta*, 258, 145–159.

[256] J.H. Flynn (1997) The 'temperature integral' – Its use and abuse. *Thermochimica Acta*, 300, 83–92.

[257] F.J. Gotor, J.M Criado, J. Malek and N. Koga (2000) Kinetic analysis of solid-state reactions: The universality of master plots for analyzing

isothermal and nonisothermal experiments. *Journal of Physical Chemistry*, 104, 10777–10782.

[258] H. Tanaka (1995) Thermal analysis and kinetics of solid state reactions. *Thermochimica Acta*, 267, 29–44.

[259] H. Tanaka, N. Koga and J. Šesták (1992) Thermoanalytical kinetics for solid state reactions as exemplified by thermal dehydration of $Li_2SO_4.H_2O$. *Thermochimica Acta*, 203, 203–220.

[260] J. Málek (1992) The kinetic analysis of non-isothermal data. *Thermochimica Acta*, 200, 257–269.

[261] N. Koga (1994) A review of the mutual dependence of Arrhenius parameters evaluated by the thermoanalytical study of solid-state reactions: |he kinetic compensation effect. *Thermochimica Acta*, 244, 1–20.

[262] A.K. Galwey (2003) Eradicating erroneous Arrhenius arithmetic. *Thermochimica Acta*, 399, 1–29.

[263] R.K. Agrawal (1992) Analysis of non-isothermal reaction kinetics. Part 1. Simple reactions. *Thermochimica Acta*, 203, 93–110.

[264] R.E. Lyon (1997) An integral method of nonisothermal kinetic analysis. *Thermochimica Acta*, 297, 117–124.

[265] A.K. Galwey (2003) Perennial problems and promising prospects in the kinetic analysis of nonisothermal rate data. *Thermochimica Acta*, 407, 93–103.

[266] S. Vyazovkin (2000) Kinetic concepts of thermally simulated reactions in solids: A view from a historical perspective. *International Reviews in Physical Chemistry*, 19, 45–60.

[267] S. Vyazovkin (2000) On the phenomenon of variable activation energy for condensed phase reactions. *New Journal of Chemistry*, 24, 913–917.

[268] A.K. Galwey (2006) What theoretical and/or chemical significance is to be attached to the magnitude of an activation energy determined for a solid-state composition? *Journal of Thermal Analysis and Calorimetry*, 86, 267–286.

[269] A.K. Galwey (2003) What is meant by the term 'variable activation energy' when applied to the kinetic analyses of solid state decompositions (crystolysis reactions)? *Thermochimica Acta*, 397, 249–268.

[270] B.V. L'vov (2001) The physical approach to the interpretation of the kinetics and mechanisms of thermal decomposition of solids: The state of the art. *Thermochimica Acta*, 373, 97–124.

[271] H.L. Anderson, A. Kemmler, G.W.H. Höhne, K. Heldt and R. Strey (1999) Round robin test on the kinetic evaluation of a complex solid state reaction from 13 European laboratories. Part 1. Kinetic TG-analysis. *Thermochimica Acta*, 332, 33–53.

[272] M.E Brown, M. Maciejewski, S. Vyazovkin, R. Nomen, J. Sempere, A. Burnham, J. Opfermann, R. Strey, H.L. Anderson, A. Kemmler, R. Keuleers, J. Janssens, H.O. Desseyn, C.-R. Li, T.B. Tang, B. Roduit, J. Malek and T. Mitsuhashi (2000) Computational aspects of kinetic analysis. Part A: The ICTAC kinetics project – Data, methods and results. *Thermochimica Acta*, 355, 125–143.

[273] N. Koga and J.M. Criado (1997) Influence of the particale size distribution on the CRTA curves for the solid-state reactions of interface shrinkage type. *Journal of Thermal Analysis and Calorimetry*, 49, 1477–1484.

[274] N. Koga and J.M. Criado (1998) Kinetic analyses of solid-state reactions with a particle-size distribution. *Journal of the American Ceramic Society*, 81, 2901–2909.

[275] A.K. Burnham and R.L. Braun (1999) Global kinetic analysis of complex materials. *Energy & Fuels*, 13, 2–22.

[276] T. Pakula, A. Tracz, G. Wegner and J.P. Rabe (1993) Kinetics of surface roughening via pit growth during the oxidation of the basal plane of graphite. II. Theory and simulation. *Journal of Chemical Physics*, 99, 8162–8167.

[277] A. Tracz, G. Wegner and J.P. Rabe (1993) Kinetics of surface roughening via pit growth during the oxidation of the basal plane of graphite. I. Experiments. *Langmuir*, 9, 3033–3038.

[278] H. Badenhorst, B. Rand and W.W. Focke (2009) Modelling of natural graphite oxidation using thermal analysis techniques. *Journal of Thermal Analysis and Calorimetry*, 99, 211–228.

[279] J.A. Hedley and D.R. Ashworth (1961) Imperfections in natural graphite. *Journal of Nuclear Materials*, 4, 70–78.

[280] F. Atamny and A. Baiker (1998) Investigation of carbon-based catalysts by scanning tunneling microscopy: Opportunities and limitations. *Applied Catalysis A: General*, 173, 201–230.

[281] A. Kavanagh and R. Schlogel (1988) The morphology of some natural and synthetic graphites. *Carbo*n, 26, 23–32.

[282] W. Jiang, G. Nadeau, K. Zaghib and K. Kinoshita (2000) Thermal analysis of the oxidation of natural graphite – The effect of particle size. *Thermochimica Acta*, 351, 85–93.

[283] K. Zaghib, G. Nadeau and K. Kinoshita (2000) Effect of graphite particle size on irreversible capacity loss. *Journal of the Electrochemical Society*, 147, 2110–2115.

[284] Y.-S. Lim, S.-H. Chi and K.-Y. Cho (2008) Change of properties after oxidation of IG-11 graphite by air and CO_2 gas. *Journal of Nuclear Materials*, 374, 123–128.

[285] M. Warrier, R. Schneider, E. Salonen and K. Nordlund (2006) Multi-scale modeling of hydrogen isotope transport in porous graphite. *Journal of Plasma Physics*, 72, 799–804.

[286] R. Schneider, A. Rai, A. Mutzke, M. Warrier, E. Salonen and K. Nordlund (2007) Dynamic Monte Carlo modeling of hydrogen isotope reactive-diffusive transport in porous graphite. *Journal of Nuclear Materia*ls, 367, 1238–1242.

[287] M. Warrier, R. Schneider, E. Salonen and K. Nordlund (2007) Effect of the porous structure of graphite on atomic hydrogen diffusion and inventory. *Nuclear Fusion*, 47, 1656–1663.

[288] S.-H. Chi, C.I. Contescu and T.D. Burchell (2008) Density change of an oxidized nuclear graphite by accoustic microscopy and image processing. *Proceedings of the 4th International Topical Meeting on High Temperature Reactor Technology*, 28 September – 1 October, Washington, DC, US.

[289] C. Berre, S.L. Fok, P.M. Mummery, J. Ali, B.J. Marsedn, T.J. Marrow and G.B. Neighbour (2008) Failure analysis of the effects of porosity in thermally oxidised nuclear graphite using finite element modelling. *Journal of Nuclear Materials*, 381, 1–8.

[290] S. Junpirom, D.D. Do, C. Tangsathitkulchai and M. Tangsathitkulchai (2005) A carbon activation model with application to logan seed char gasification. *Carbon*, 43, 1936–1943.

[291] T.S. Ong and H. Yang (2000) Effect of atmosphere on the mechanical milling of natural graphite. *Carbon*, 38, 2077–2085.

[292] A. Touzik, M. Hentsche, R. Wentzel and H. Hermann (2006) Effect of mechanical grinding in argon and hydrogen atmosphere on microstructure of graphite. *Journal of Alloys and Compounds*, 426, 272–276.

[293] P.L. Walker, Jr., M. Shelef and R.A. Anderson (1968) Catalysis of carbon gasification. In: *Chemistry and Physics of Carbon,* Vol. 4, Marcel Dekker, New York.

[294] O.C. Kopp, E.L. Fuller Jr and A.D. Surrett (1993) The effect of trace elements on the surface oxidation of H-451 graphite. *Journal of Nuclear Materials*, 207, 333–338.

[295] D.W. McKee (1981) The catalyzed gasification reactions of carbon. In: *Chemistry and Physics of Carbon*, Vol. 16, Marcel Dekker, New York.

[296] D.W. McKee and D. Chatterji (1975) The catalytic behaviour of alkali metal carbonates and oxides in graphite oxidation reactions. *Carbon*, 13, 381–390.

[297] R.T.K. Baker, C.R.F. Lund and J.J. Chludzinski Jr (1984) Catalytic gasification of graphite by barium in steam, carbon dioxide, oxygen and hydrogen. *Journal of Catalysis*, 87, 255–264.

[298] R.T.K. Baker, R.B. Thomas and M. Wells (1975) Controlled atmosphere electron microscopy studies of graphite gasification. The catalytic influence of vanadium and vanadium pentoxide. *Carbon*, 13, 141–145.

[299] R.T.K. Baker, P.S. Harris, D.J. Kemper and R.J. Waite (1974) Controlled atmosphere electron microscopic studies of the catalysed graphite-oxygen reaction. 3. The catalytic influence of molybdenum and molybdenum trioxide. *Carbon,* 12, 179–187.

[300] R.T. Yang and C. Wong (1984) Catalysis of carbon oxidation by transition metal carbides and oxides. *Journal of Catalysis*, 85, 154–168.

[301] R.T.K. Baker and R.D. Sherwood (1981) Catalytic gasification of graphite by nickel in various gaseous environments. *Journal of Catalysis*, 70, 198–214.

[302] R.T.K. Baker, J.J. Chludcinski Jr and and R.D. Sherwood (1985) A comparison of the catalytic influence of nickel, iron and nickel-iron on the gasification of graphite in various gaseous environments. *Carbon*, 23, 245–254.

[303] R.T.K. Baker and J.J. Chludzinski Jr (1981) Catalytic gasification of graphite by chromium and copper in oxygen, steam and hydrogen. *Carbon*, 19, 75–82.

[304] D.W. McKee (1970) The copper-catalyzed oxidation of graphite. *Carbon*, 8, 131–139.

[305] P.S. Harris and F.S. Feates (1974) Controlled atmosphere electron microscopy studies of graphite gasification. 4. Catalysis of the graphite-O_2 reaction by silver. *Carbon*, 12, 189–197.

[306] R.T.K. Baker, J.A. France, L. Rouse and R.J. Waite (1976) Catalytic oxidation of graphite by platinum and palladium. *Journal of Catalysis*, 41, 22–29.

[307] P.S. Harris, F.S. Feates and B.G. Reuben (1973) Controlled atmosphere electron microscopic studies of the catalysed graphite-oxygen reaction. 2. The influence of lead. *Carbon*, 11, 565–566.

[308] C. Roscoe (1968) Catalytic oxidation of Ticonderoga graphite crystals. *Carbon*, 6, 365–372.

[309] A. Tomita and Y. Tamai (1972) Hydrogenation of carbons catalyzed by transition metals. *Journal of Catalysis*, 27, 293–300.

[310] A. Tomita and Y. Tamai (1974) An optical microscopic study on the catalytic hydrogenation of graphite. *Journal of Physical Chemistry*, 78, 2254–2258.

[311] C.W. Keep, S. Terry and M. Wells (1980) Studies of the nickel-catalyzed hydrogenation of graphite. *Journal of Catalysis*, 66, 451–462.

[312] P.J. Goethel and R.T. Yang (1986) Platinum-catalyzed hydrogenation of graphite: mechanism studied by the rates of monolayer channeling. *Journal of Catalysis*, 101, 342–351.

[313] S.G. Chen and R.T. Yang (1992) Mechanism of alkali and alkaline earth catalyzed gasification of graphite by CO_2 and H_2O studied by electron microscopy. *Journal of Catalysis*, 138, 12–23.

[314] Z.J. Pan and R.T. Yang (1991) Catalytic behavior of transition metal oxide in graphite gasification by oxygen, water and carbon dioxide. *Journal of Catalysis*, 130, 161–172.

[315] X. Chu, L.D. Schmidt, S.G. Chen and R.T. Yang (1993) Catalyzed carbon gasification studied by scanning tunneling microscopy and atomic force microscopy. *Journal of Catalysis*, 140, 543–556.

[316] H.Y. Huang and R.T. Yang (1999) Catalyzed carbon-NO reaction studied by scanning tunnling microscopy and *ab initio* molecular orbital calculations. *Journal of Catalysis*, 185, 286–296.

[317] S. Konishi, W. Sugimoto, Y. Murakami and Y. Takasu (2006) Catalytic reaction of channels in the surface layers of highly oriented pyrolytic graphite by cobalt nanoparticles. *Carbon*, 44, 2330–2356.

[318] G.R. Hennig (1962) Catalytic oxidation of graphite. *Journal of Inorganic Nuclear Chemistry*, 24, 1129–1137.

[319] H. Harker, J.B. Horsley and D. Robson (1970) The reactivity of graphite to oxygen: the effect of impurities added after neutron-irradiation. *Journal of Nuclear Materials*, 37, 331–339.

[320] A.E.B. Presland and J.A. Hedley (1963) An electron microscope study of the thermal oxidation of natural graphite. *Journal of Nuclear Materials*, 10, 99–112.

[321] D.W. McKee (1970) Metal oxides as catalysts for the oxidation of graphite. *Carbon*, 8, 623–635.

[322] R.T.K. Baker (1979) In situ electron microscopy studies of catalyst particle behaviour. *Catalysis Reviews: Science and Engineering*, 19, 161–209.

[323] R.T.K. Baker (1986) Factors controlling the mode by which a catalyst operates in the graphite-oxygen reaction. *Carbon*, 24, 715–717.

[324] S.S. Datta (2010) Wetting and energetics in nanoparticle etching of graphene. *Journal of Applied Physics*, 108, 243071–243077.

[325] X. Wu and L.R. Radovic (2005) Catalytic oxidation of carbon/carbon composite materials in the presence of potassium and calcium acetates. *Carbon*, 43, 333–344.

[326] J.-L. Su and D.D. Perlmutter (1985) Porosity effects on catalytic char oxidation. Part II: Experimental results. *AIChE Journal*, 31, 965–971.

[327] A. Tomita (2001) Catalysis of carbon-gas reactions. *Catalysis Surveys from Japan*, 5, 17–24.

[328] P.J. Goethel and R.T. Yang (1989) Mechanism of catalyzed graphite oxidation by monolayer channeling and monolayer edge recession. *Journal of Catalysis*, 119, 201–214.

[329] S.S. Datta, D.R. Strachan, S.M. Khamis and A.T.C. Johnson (2008) Crystallographic etching of few-layer graphene. *Nano Letters*, 8, 1912–1915.

[330] L. Ci, L. Song, D. Jariwala, A.L. Elias, W. Gao, M. Terrones and P.M. Ajayan (2009) Graphene shape control by multistage cutting and transfer. *Advanced Materials*, 21, 4487–4491.

[331] N. Severin, S. Kirstein, I.M. Sokolov and J.P. Rabe (2009) Rapid trench channeling of graphenes with catalytic silver nanoparticles. *Nano Letters*, 9, 457–461.

[332] L.P. Biro and P. Lambin (2010) Nanopatterning of graphene with crystallographic orientation control. *Carbon*, 48, 2677–2689.

[333] F. Schaffel, J.H. Warner, A. Bachmatiuk, B. Rellinghaus, B. Buchner, L. Schultz and M.H. Rummeli (2009) Shedding light on the crystallographic etching of multi-layer graphene at the atomic scale. *Nano Research*, 2, 695–705.

[334] L. Ci, Z. Xu, L. Wang, W. Gao, F. Ding, K.F. Kelly, B.I. Yakobson and P.M. Ajayan (2008) Controlled nanocutting of graphene. *Nano Research*, 1, 116–122.

[335] C. Heuchamps and X. Duval (1966) Effet des catalyseurs sur les caracteristiques cinetiques de la combustion du graphite. *Carbon*, 4, 243–253.

[336] F.S. Feates, P.S. Harris and B.G Reuben (1974) Compensation effect in the kinetics of catalysed oxidation of carbon. *Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases*, 70, 2011–2020.

[337] A.S. Choi, A.L. Devera and Hawlay M.C (1987) A mathematical model of the chanelling activity of metal particles during a catalyzed oxidation of graphite. *Journal of Catalysis*, 106, 313–317.

[338] P.J. Goethel, J.A. Tsamopoulos and R.T. Yang (1989) Modeling the channeling action of catalysts in gas-carbon reactions. *AIChE Journal*, 35, 686–689.

[339] L. Li, Z.-C. Tan, S.-H. Meng, S.-D. Wang and D.-Y. Wu (2000) Kinetic study of the accelerating effect of coal-burning additives on the combustion of graphite. *Journal of Thermal Analysis and Calorimetry*, 62, 681–685.

[340] J.M. Ranish and P.L. Walker Jr (1990) Models for roughening of graphite during its catalyzed gasification. *Carbon*, 28, 887–896.

[341] D.W. McKee (1991) Oxidation protection of carbon materials. In: *Chemistry and Physics of Carbon*, Vol. 23, Marcel Dekker, New York.

[342] Q. Wang, X.-L. Ma, L.-Q. Chen, W. Cermignani and C.G. Pantano (1997) Effect of boron on graphite oxidation – A theoretical study. *Carbon*, 35, 307–313.

[343] A.P. Wieber, J.E. Guzman and E.E. Wolf (2006) An STM study of phosphoric acid inhibition of the oxidation of HOPG and carbon catalyzed by alkali salts. *Carbon*, 44, 2069–2079.

[344] C. Palache (1941) Contributions to the minerology of Sterling Hill, New Jersey: Morphology of graphite, aresenopyrite, pyrite and arsenic. *American Mineralogist*, 26, 709–717.

[345] H. Badenhorst, B. Rand and W.W. Focke (2011) Geometric effects control isothermal oxidation of graphite flakes. Submitted to *Journal of Thermal Analysis and Calorimetry*.