

Bibliography

- [1] K. Domen T. Arai, K. Maruya and T. Onishi, *Journal of Catalysis*, **141**, 533, 1993.
- [2] K. Maruya C. Li, K. Domen and T. Onishi, *Journal of Catalysis*, **141**, 540, 1993.
- [3] W. Göpel, *Cryst. Latt. Def. and Amorph. Mat*, **18**, 315, 1989.
- [4] H. L. Tuller and A. S. Nowick, *J. Electrochem. Soc.*, **122**, 255, 1975.
- [5] P. Kofstad, *Non-stoichiometry, Diffusion and Electrical Conductivity in Binary Metal Oxides*. Wiley Interscience, New York, 1972.
- [6] H. L. Tuller and A. S. Nowick, *J. Phys. Chem. Solids*, **38**, 859, 1977.
- [7] H. L. Tuller and A. S. Nowick, *J. Electrochem. Soc.*, **126**, 209, 1979.
- [8] K. Eguchi H. Yahiro and H. Arai, *Solid State Ionics*, **36**, 71, 1989.
- [9] G. B.Balazs and R. S. Glass, editors, *Ionic and Mixing Conducting Ceramics, 2nd International Symposium*, page 478.
- [10] P. L. Chen and I. W. Chen, *J. Am. Ceram. Soc.*, **77**, 2289, 1994.

- [11] B. E. F. Fender V. Butler, C. R. A. Catlow and J. H. Harding, *Solid State Ionics*, **8**, 109, 1983.
- [12] S. E. Hill and C. R. A. Catlow, *J. Phys. Chem. Solids*, **54**, 411, 1993.
- [13] T. Mukoyama H. Nakamatsu and H. Adachi, *Chem. Phys. Lett.*, **247**, 168, 1995.
- [14] H. C. Yao and Y. F. Yu Yao, *Journal of Catalysis*, **86**, 254, 1984.
- [15] C. N. Monteruil E. C. Su and W. G. Rothschild, *Applied Catalysis*, **17**, 75, 1985.
- [16] E. C. Su and Rothschild, *Journal of Catalysis*, **99**, 506, 1986.
- [17] J. C. Summers and S. A. Ausen, *Journal of Catalysis*, **58**, 131, 1979.
- [18] G. J. Mains T. Jin, T. Okuhara and J. M. White, *J. Phys. Chem.*, **91**, 3310, 1987.
- [19] G. J. Mains T. Jin, Y. Zhou and J. M. White, *J. Phys. Chem.*, **91**, 5931, 1987.
- [20] A. F. Diwell B. Harrison and C. Hallet, *Platinum Metals Rev.*, **32**, 73, 1988.
- [21] C. Hardacre R. M. Ormerod and R. M. Lambert, *J. Phys. Chem.*, **98**, 10901, 1994.
- [22] R. R. Rajaram S. E. Golunski, H. A. Hatcher and T. J. Truex, *Applied Catalysis B*, **5**, 367, 1995.
- [23] M. Wolcyrz L. Kepinski and J. Okal, *J. Chem. Soc. Faraday Trans.*, **91**, 507, 1995.

- [24] F. Stephanopoulos A. Tschoper, W. Liu and J. Y. Ying, *Journal of Catalysis*, **in press**, 1996.
- [25] A. J. Tench M. Dufaux M. Che, J. F. J. Kibblewhite and C. Naccache, *J. Chem. Soc. Faraday Trans.*, **69**, 857, 1973.
- [26] S. C. Parker T. X. T. Sayle and C. R. A. Catlow, *Surf. Sci.*, **316**, 329, 1993.
- [27] T. X. T. Sayle. PhD thesis, University of Bath, 1993.
- [28] S. C. Parker T. X. T. Sayle and C. R. A. Catlow, *J. Phys. Chem.*, **98**, 13625, 1994.
- [29] N. W. Cant C. Padeste and D. L. Trimm, *Catalysis Letters*, **18**, 305, 1993.
- [30] J. Z. Shyu and K. Otto, *Journal of Catalysis*, **115**, 16, 1989.
- [31] W. L. H. Watkins G. W. Graham R. K. Belitz J. Z. Shyu, K. Otto and H. S. Gandhi, *Journal of Catalysis*, **114**, 23, 1988.
- [32] T. Shido and Y. Iwasawa, *Journal of Catalysis*, **136**, 493, 1992.
- [33] T. Shido and Y. Iwasawa, *Journal of Catalysis*, **141**, 71, 1993.
- [34] W. D. J. Evans B. J. Cooper and B. Harrison, *Catalysis and Automotive Pollution Control*, page 117. Elsevier Science, Amsterdam, 1987.
- [35] A. H. Harker and R. W. Grimes, *Special Issue of Mol. Sim.*, **4** [5], 1990.
- [36] A. H. Harker and R. W. Grimes, *Special Issue of Mol. Sim.*, **5** [2], 1990.
- [37] C. R. A. Catlow and W. C. Mackrodt, editors, *Computer Simulation of Solids*. Springer-Verlag, Berlin, 1982.

- [38] C. R. A. Catlow and A. M. Stoneham, *Special Issue of J. Chem. Soc. Faraday Trans.*, **85** [5], 1989.
- [39] I.M. Boswarva and A. L. Lidiard, *Phil. Mag.*, **16**, 805, 1967.
- [40] K. M. Diller P. W. Jacobs C. R. A. Catlow, J. Corish and M. J. Norgett, *J. Phys.:C*, **12**, 451, 1979.
- [41] M. J. Norgett and A. B. Lidiard, *Phil. Mag. B*, **18**, 1193, 1968.
- [42] M. J. Norgett C. R. A. Catlow and T. A. Ross, *J. Phys. C.: Solid State Phys*, **10**, 1627, 1977.
- [43] M. S. Islam and C. Ananthamoham, *Phys. Rev. B*, **44**, 9492, 1991.
- [44] X. Zhang and C. R. A. Catlow, *J. Mater. Chem*, **1**, 233, 1991.
- [45] C. R. A. Catlow, *Phil. Trans. R. Soc. London. A.*, **341**, 255, 1992.
- [46] R. A. Jackson and C. R. A. Catlow, *Mol. Simul.*, **1**, 207, 1988.
- [47] W. C. Mackrodt, *Advances in ceramics*, volume 10, page 62. American Ceramic Society, Westerville, Ohio, 1984.
- [48] R. W. Grimes, *J. Am. Ceram. Soc.*, **77**, 378, 1994.
- [49] G. D. Price R. Ferneyhough, D. Fincham and M. J. Gillian, *Modelling Simul. Mater. Sci. Eng.*, **2**, 1101, 1994.
- [50] A. Dornford-Smith and R. W. Grimes, *Phil. Mag B.*, **72**, 563, 1995.
- [51] D. W. Lewis and C. R. A. Catlow, *Topics in Catalysis*, **1**, 111, 1994.

- [52] C.R.A. Catlow A.R. George and J.M. Thomas, *J. Chem. Soc. Faraday Trans.*, **91**, 3975, 1995.
- [53] J. D. Gale, *GULP, The Royal Institution of Great Britain*, 1995.
- [54] C. Young and D. Wills, *Ray Tracing Creations, 2nd Edition*. Waite Group Press, 1994.
- [55] P. W. Tasker, *J. Phys.: C*, **12**, 4977, 1979.
- [56] P. W. Tasker and D. M. Duffy, *Surf. Sci.*, **137**, 97, 1984.
- [57] W. C. Mackrodt and R. F. Stewart, *J. Phys.:C*, **12**, 5015, 1979.
- [58] J. Purton P. M. Oliver, S. C. Parker and D. W. Bullett, *Surf. Sci.*, **307**, 1200, 1994.
- [59] D.J.Binks. PhD thesis, University Of Surrey, 1994.
- [60] S. C. Parker P. M. Oliver and W. C. Mackrodt, *Modelling Simul. Mater. Sci. Eng.*, **1**, 755, 1993.
- [61] D. H. Gay C. R. A. Catlow R. J. Davey N. L. Allan, A. L. Rohl and W. C. Mackrodt, *Faraday Discuss.*, **95**, 273, 1993.
- [62] A.L. Rohl A.R. George, K.D.M. Harris and D.H. Gay, *J. Mat. Chem.*, **5**, 133, 1995.
- [63] D. C. Sayle. PhD thesis, University of Bath, 1992.
- [64] S. C. Parker D. C. Sayle and J. H. Harding, *Mol. Simul.*, **12**, 127, 1994.

- [65] S. C. Parker D. C. Sayle and J. H. Harding, *Phil. Mag. A*, **69**, 787, 1994.
- [66] D. H. Gay A. L. Shluger, A. L. Rohl and R. T. Williams, *J. Phys. Condens. Matter*, **6**, 1825, 1994.
- [67] C. R. A. Catlow, *Special Issue of J. Mater. Chem.*, **4**, 793, 1994.
- [68] C. R. A. Catlow, *Computational Materials Science*, **2**, 6, 1994.
- [69] M. Born and J. E. Mayer, *Z. Physik.*, **75**, 1, 1932.
- [70] D. J. Tildesley and M. P. Allen, *Computer Simulation of Liquids*, 2nd Edition. Clarendon Press, Oxford, 1989.
- [71] K. Chan S. Y. Liem and R. F. Savinell, *Mol. Sim.*, **13**, 47, 1994.
- [72] D. J. Binks R. W. Grimes and A. B. Lidiard, *Phil. Mag. A*, **72** [3], 1995.
- [73] R. G. Gordon and Y. S. Kim, *J. Chem. Phys.*, **56**, 3122, 1972.
- [74] P. T. Wedepohl, *Proc. Phys. Soc.*, **92**, 79, 1967.
- [75] J. H. Harding and A. H. Harker, in “AERE R10425”. Harwell Laboratory, 1982.
- [76] R. W. Grimes. PhD thesis, University Of Keele, 1988.
- [77] P. J. Knowles P. W. Fowler and N. C. Pyper, *Mol. Phys.*, **56**, 83, 1985.
- [78] J. D. Gale A. Jentys, R. W. Grimes and C. R. A. Catlow, *J. Phys. Chem.*, **97**, 13535, 1993.
- [79] B. G. Dick and A. W. Overhauser, *Phys. Rev.*, **112**, 90, 1958.

- [80] R. G. Ball, *in “AEA-RS2127”*. Harwell Laboratory, 1991.
- [81] C. R. A. Catlow, *Proc. Roy. Soc. Lond. A*, **353**, 1977, 1989.
- [82] P. P. Ewald, *Ann. Physik.*, **64**, 253, 1921.
- [83] C. R. A. Catlow and M. J. Norgett, *in “AERE-M2936”*. Harwell Laboratory, 1976.
- [84] C. Kittel, *Introduction To Solid State Physics, 6th Edition*. J. Wiley and sons, New York, 1986.
- [85] S. A. Teukolsky W. H. Press, B. P. Flannery and W. T. Vetterling, *Numerical Recipes, The Art of Scientific Computing*. Cambridge University Press, 1988.
- [86] R. Fletcher, *Practical Methods of Optimisation*, volume 1. J. Wiley and sons, New York, 1980.
- [87] R. Fletcher and M. J. Powell, *Computant J.*, **6**, 163, 1963.
- [88] N. F. Mott and M. J. Littleton, *Trans. Farad. Soc.*, **34**, 485, 1938.
- [89] M. Leslie, *in “Report DL/SCI/TM31T”*. SERC Daresbury Laboratory, 1982.
- [90] D. E. Parry, *Surf. Sci.*, **49**, 433, 1975.
- [91] D. E. Parry, *Surf. Sci.*, **54**, 195, 1975.
- [92] M. Barber D.M. Heyes and J.H.R. Clarke, *J. Chem. Soc. Faraday Trans.*, **73**, 1485, 1977.
- [93] J. H. Harding, *in “AERE-R14300”*. Harwell Laboratory, 1988.

- [94] P. W. Tasker, *in “AERE-R9130”*. Harwell Laboratory, 1978.
- [95] D. H. Gay and A. L. Rohl, *J. Chem. Soc. Farad. Trans.*, **91**, 925, 1995.
- [96] A. Rahman, *Phys. Rev. A.*, **136**, 405, 1964.
- [97] G. D. Harp and B. J. Berne, *J. Chem. Phys.*, **49**, 1249, 1968.
- [98] C. W. Gear, *in “Report ANL-7126”*. Argonne National Laboratory, 1966.
- [99] C. W. Gear, *Numerical initial value problems in ordinary differential equations*. Prentice-Hall, 1971.
- [100] H. Fuchs J. A. Gardner W. E. Evenson H. T. Su, R. Wang and J. A. Summers, *J. Am. Ceram. Soc.*, **73**, 3215, 1990.
- [101] W. E. Evenson R. Wang, J. A. Gardner and J. A. Sommers, *in Point Defects and Related Properties of Ceramics*, volume 24. The American Ceramic Society, Westerville, OH, 1991.
- [102] W. E. Evenson R. Wang, J. A. Gardner and J. A. Sommers, *in Proceedings of the XII International Conference on Defects in Insulating Materials*, volume 2. World Scientific, Singapore, 1993.
- [103] W. E. Evenson R. Wang, J. A. Gardner and J. A. Sommers, *Phys. Rev. B*, **47**, 638, 1993.
- [104] C. R. A. Catlow A. N. Cormack and A. S. Nowick, *J. Phys. Chem. Solids*, **50**, 177, 1989.
- [105] A. Yoshihara A. Nakajima and M. Ishigame, *Phys. Rev. B.*, **50**, 13297, 1994.

- [106] R. D Shannon, *Acta. Ctystrallogr. A*, **32**, 751, 1976.
- [107] S. Vyas, R. W. Grimes, D. H. Gay, and A. L . Rohl, *J. Chem. Soc. Farad. Trans.*, **94**, 427, 1998.
- [108] W. D. Kingery, editor, *Advances in ceramics: Structure and properties of MgO and Al₂O₃ ceramics*, volume 10. 1984.
- [109] P. G. Ribbe A. M. Alper, R. N. McNally and R. C.Doman, *J. Am. Ceram. Soc.*, **45**, 264, 1962.
- [110] T. Endo T. Sato, K. Kato and M. Shimada, *Reactivity of Solids*, **2**, 253, 1986.
- [111] V. Fornés F. Rey and J. M. Rojo, *J. Chem. Soc. Faraday Trans.*, **88**, 2233, 1992.
- [112] C. L. Rohrer and G. S.Rohrer, *Chem. Mater.*, **6**, 501, 1994.
- [113] L. Pauling, *J. Am. Chem. Soc.*, **51**, 1010, 1929.
- [114] P. W. M. Jacobs C. R. A. Catlow, J. Corish and A. B. Lidiard, *J. Phys.: C*, **14**, 121, 1981.
- [115] C. G. Kinniburgh and J. A. Walker, *Surf. Sci.*, **63**, 274, 1977.
- [116] M. R. Welton-Cook and W. Berndt, *J. Phys.: C*, **15**, 5691, 1982.
- [117] S. R. Morrison, *The Chemical Physics of Surfaces*. Plenum, New York, 1990.
- [118] T. E. Mitchell D. H. Gay S. Vyas M. Yan, S. P. Chen and R. W. Grimes, *Phil. Mag. A*, **72**, 121, 1995.

- [119] F. Bertant, *Compt. Rendu*, **246**, 3447, 1958.
- [120] J. A. Kilner. *Private Communication*. 1995.
- [121] L. Gerward and J. Staun-Olsen, *Powder Diffraction*, **8**, 127, 1993.
- [122] J. W. Gibbs, *Collected Works*. Longman, New York, 1928.
- [123] P. Hartman and P. Bennema, *J. Cryst. Growth*, **49**, 145, 1980.
- [124] P. W. Atkins, *Physical Chemistry, 3rd Edition*, page 765. Oxford University Press, 1986.
- [125] B. M. Wanklyn and B. J. Garrard, *J. Cryst. Growth*, **66**, 346, 1984.
- [126] B. M. Wanklyn. *Private Communication*. 1994.
- [127] J. Goniakowsk and C. Nogurera, *Surf. Sci.*, **323**, 129, 1995.
- [128] R. D. King-Smith M. Ramamoorthy and David Vanderbilt, *Phys. Rev. B*, **49**, 7709, 1994.
- [129] R. D. King-Smith M. Ramamoorthy and David Vanderbilt, *Phys. Rev. B*, **49**, 16721, 1994.
- [130] V. L. Bulatov A. Dornford-Smith and R. W. Grimes, *Ceramic Transactions*, **in press**, 1996.
- [131] H. Edelsbrunner and E. P. Mücke, *ACM Transactions on Graphics*, **13**, 43, 1994.
- [132] R. C. Weast, *C. R. C. Handbook of Chemistry and Physics, 69th Edition*. C. R. C. Press, Boca Raton, Florida, 1989.

- [133] M. Amini and R. W. Hockney, *J. Non-Cryst. Solids*, **31**, 447, 1979.
- [134] D. Fincham M. Amini and R. W. Hockney, *J. Phys.:C*, **12**, 4707, 1979.
- [135] A. H. Harker. *Private Communication*. 1996.