Bibliography

[1] Hammond C 1997 *The Basics of Crystallography and Diffraction*. Oxford University Press.

[2] Frenkel J 1926 *Zeitschrift für Physik* **35** 652.

[3] Schottky W and Wagner C 1930 *Zeitschrift für Physikalische Chemie* **11B** 335.

[4] Schottky W 1935 *Zeitschrift für Physikalische Chemie* **29B** 335.

[5] Stirling J 1730 *Methodus Differentialis*. London.

[6] Chiang Y M Birnie III D and Kingery W D 1997 *Physical Ceramics*. John Wiley & Sons.

[7] Debye P and Huckel E 1923 *Physikalische Zeitschrift* **24** 185.

[8] Debye P and Huckel E 1924*Physikalische Zeitschrift* **25** 185.

[9] Allnatt A R, Pantelis P and Sime S J 1971. *Journal of Physics C: Solid State Physics* **4** 1778.

[10] Yuen P S and Allnatt A R 1975 *Journal of Physics C: Solid State Physics* **8** 2213.

[11] Wagner C 1977 *Annual Review of Materials Science* **7** 1

[12] Zacate M O and Grimes R W 2002 *Journal of the Physics and Chemistry of Solids* **63** 675

[13] Stanek C R and Grimes R W 2002 *Journal of the American Ceramic Society* **85** 2139.

[14] Rushton M J D, Grimes R W, Stanek C R and Owens S 2004 *Journal of Materials Research* **19** 1603.

[15] Todorov I T, Allan N L, Lavrentiev M Yu, Freeman C L, Mohn C E and Purton J A 2004 *Journal of Physics: Condensed Matter* **16** 2751.

[16] Fick A E 1855 *Annalen der Physik und Chemie* **94** 59.

[17] Shewmon P 1989 *Diffusion in Solids* 2nd ed. The Minerals, Metals and Materials Society.

[18] Bragg W H 1915 *Philosophical Magazine* **30** 305.

[19] Nishikawa S 1915 *Proceedings of the Mathematical Physics Society of Tokyo* **8** 199.

[20] Barth T F W and Posnjak E 1931 *Journal of the Washington Academy of Sciences* **21** 255.

[21] Posnjak E and Barth T F W 1931 *Physical Review* **38** 2234.

[22] Barth T F W and Posnjak E 1932 *Zeitschrift für Kristallographie* **82** 325.

[23] Verwey E J W and Heilmann E L 1947 *Journal of Chemical Physics* **15** 174.

[24] Brun E and Hafner S 1962 *Zeitschrift für Kristallographie* **117** 37.

[25] Brun E and Hafner S 1962 *Zeitschrift für Kristallographie* **117** 63.

[26] Gobbi G C, Christoffersen R, Otten M T, Miner B, Buseck P R, Kennedy G J and Fyfe C A 1985 *Chemistry Letters* **6** 771.

[27] Millard R L Peterson R C and Hunter B K *American Mineralologist* 1992 **77** 44

[28] Hafner S and Laves F 1961 *Zeitschrift für Kristallographie* **115** 321.

[29] Hafner S 1961 *Zeitschrift für Kristallographie* **115** 331.

[30] Stoll E, Fischer P, Hälg W and Maier G 1964 *Journal of Physics, Paris* **25** 447.

[31] Bacon G E 1952 *Acta Crystallographica* **5** 684.

[32] Fischer F 1967 *Zeitschrift für Kristallographie* **124** 275.

[33] Schmocker U, Boesch H R and Waldner F 1972 *Physics Letters* **40A** 237.

[34] Schmocker U and Waldner F 1976 *Journal of Physics C: Solid State Physics* **9** L235.

[35] Clinard F W, Hurley G F and Hobbs L W 1982 *Journal of Nuclear Materials* **665** 108.

[36] Tucker D S, Zocco T, Kise C D and Kennedy J C 1986 *Journal of Nuclear Materials* **401** 141.

[37] Nakai K, Fukumoto K and Kinoshita C 1992 *Journal of Nuclear Materials* **630** 191.

[38] Sickafus K E, Mills J M, Grimes N W 1999*Journal of the American Ceramic Society* **82** 3279.

[39] Sickafus K E, Larson A C, Yu N and Nastasi M 1995 *Journal of Nuclear Materials* **219** 128.

[40] Sickafus K E, Minervini L, Grimes R W, Valdez J A, Ishimaru M, Li F, McClellan K J and Hartmann T 2000 *Science* **289** 748.

[41] Ishimaru M, Hiroysu Y, Afanasyev-Charkin I V and Sickafus K E 2002 *Journal of Physics: Condensed Matter* **14** 1237.

[42] Tuller H L and Nomick A S 1979 *Journal of the Electrochemical Society* **126** 209.

[43] Blumenthal R N, Brugner F S and Garnier J E 1973 *Journal of the Electrochemical Society* **120** 1230.

[44] Tuller H L and Nomick A S 1975 *Journal of the Electrochemical Society* **122** 255.

[45] Kudo T and Obayashi H 1976 *Journal of the Electrochemical Society* **123** 415.

[46] Dristine R T, Blumenthal R N and Kuech T F 1979 *Journal of the Electrochemical Society* **126** 264.

[47] Yahiro H, Eguchi K and Arai H 1986 *Solid State Ionics* **21** 37.

[48] Faber J, Geoffroy C, Roux A, Sylvestre A and Ableard A 1989 *Applied Physics A: Solids and Surfaces* **49** 225.

[49] Balazs G B abd Glass R S 1995 *Solid State Ionics* **76** 155.

[50] Gerhard-Anderson R and Nowick A S 1981 *Solid State Ionics* **5** 547.

[51] Kilner J A and Brook R J 1982 *Solid State Ionics* **6** 237.

[52] Wang D Y, Park D S, Griffith J and Nowick A S 1981 *Solid State Ionics* **2** 95.

[53] Kröger F A and Vink H J 1957 *Solid State Physics - Advances in Research Applications* Academic Press New York

[54] Born M and Mayer J 1932 *Zeitschrift für Physik* **75** 1.

[55] Born M and Mayer J 1933 *Journal of Chemical Physics.* **1** 270.

[56] Harding J H 1990 *Reports on Progress in Physics*, **53** 1403.

[57] Bleaney B I and Bleaney B 1968 *Electricity and magnetism.* page 33. Oxford University Press, 2nd Edition.

[58] Allen M P and Tildesley D J 1987 *Computer Simulation of Liquids*. Clarendon Press, Oxford.

[59] Ewald P P 1921 *Annalen der Physik* **64** 253.

[60] Kittel C 1996 *Introduction to Solid State Physics*. John Wiley & Sons. New York, 7th Edition.

[61] Catlow C R A and Norgett M J 1976 Technical Report AERE-M2936, Harwell Laboratory.

[62] Buckingham R A 1938 *Proceedings of the Royal Society A*, **168** 264.

[63] Vail J M, Harker A H, Harding J H and Saul P 1984 *J. Phys. C: Solid State Physics*, **17** 3401.

[64] Lewis G V and Catlow C R A 1985 *J. Phys. C: Solid State Physics*, **18**, 1149.

[65] Tarento R J and Harding J H 1987 *Journal of Physics C: Solid State Physics*, **20** L677

[66] Cormack A N and Parker S C 1990 *Journal of the American Ceramic Society*, **73** 3220.

[67] Minervini L, Zacate M O and Grimes R W 1999 *Solid State Ionics*, **116** 339.

[68] Minervini L, Grimes R W and Sickafus K E 2000 *Journal of the American Ceramic Society* **83** 1873.

[69] Zacate M O and Grimes R W 2000 *Philosophical Magazine A*, **80** 797.

[70] Levy M R, Grimes R W and Sickafus K E 2004 *Philosophical Magazine*, **84** 533.

[71] London F 1930 *Zeitschrift für Physik.* **63** 245.

[72] London F 1930 *Zeitschrift für Physikalische Chemie (B).* **11** 222

[73] Eisenschitz R and London F 1930 *Zeitschrift für Physik.* **60** 491

[74] Margenau H 1931 *Physical Review.* **38** 365

[75] Slater J C and Kirkwood J G 1931 *Physical Review.* **37** 682.

[76] Grimes N W and Grimes R W 1998 *Journal of Physics: Condensed Matter*, **10** 3029.

[77] Grimes N W and Grimes R W 1997 *Journal of Physics: Condensed Matter*, **9** 6737.

[78] Jentys A and Grimes R W 1996 *Journal of the Chemical Society, Faraday Transactions*, **92** 2093.

[79] Dick B G and Overhauser A W 1958 *Physical Review* **112** 90.

[80] Born M and Huang K 1954 *Dynamical Theory of Crystal Lattices.* Oxford University Press.

[81] Schröder U 1966 *Solid State Communications* **4** 347.

[82] Sangster M J L 1974 *Journal of Physics and Chemistry of Solids* **35** 194.

[83] Jordan D W and Smith P 1997 *Mathematical Techniques*. Oxford University Press. 2nd Edition.

[84] Mott N F and Littleton M J 1938 *Trans. Faraday Soc.* **34** 485.

[85] Newman M E J and Barkema G T 2004 *Monte Carlo Methods in Statistical Physics* Oxford University Press.

[86] Gibbs J W 1902 *Elementary Principles of Statistical Mechanics* Yale University Press.

[87] Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 *Journal of Chemical Physics* **21** 1087.

[88] Hohenburg R and Kohn W 1964 *Physical Review* **136** 864.

[89] Kohn W and Sham L J 1965 *Physical Review A* **140** 1133.

[90] Ledin L and Lundqvist B I 1971 *Journal of Physics C: Solid State Physics* **4** 2064.

[91] Jones R O and Gunnarsson O 1989 *Reviews of Modern Physics* **61** 689.

[92] Perdew J P and Yue Wang 1992 *Physical Review B*, **45** 13244.

[93] Perdew J P, Burke K and Ernzerhof M 1996 *Physical Review of Letters* **77** 3865.

[94] Coles B R and Caplin A D 1976 *The Electronic Structures of Solids*. Edward Arnold Publishers Ltd.

[95] Ashcroft N W and Mermin N D 1976 *Solid State Physics*. Harcourt Inc.

[96] Monkhorst H J and Pack J D 1976 *Physial Review B* **13** 5188.

[97] Ball J A, Pirzada M, Grimes R W, Zacate M O, Price D W and Uberuaga B P 2005 *Journal of Physics: Condensed Matter* **17** 7621.

[98] Buckley S N and Shaibani 1987 *Philosophical Magazine Letters* **55** 15

[99] Buckley S N 1986 *Journal of Nuclear Materials* **387** 141

[100] Kinoshita C and Nakai K 1989 In *Japan-France Seminar* series 2:(Lattice Defects in Ceramics, Tokyo)

[101] Sickafus K E, Hanrahan R J, McClellan K J, Mitchell J N, Wetteland C J, Butt D P, Chodak P, Ramsey K P, Blair T H, Chidester K , Matzke H, Yasuda K, Verrall R A and Yu N 1999 American Ceramic Society Bulletin **78** 69.

[102] Skvortsova V, Mironova-Ulmane N and Ulmanis U 2002 *Nuclear Instruments and Methods in Physics Research B* **191** 256.

[103] Matzke H, Rondinella V V and Wiss T 1999 *Journal of Nuclear Materials* **274** 47.

[104] Chauvin N, Konigs R J M and Matzke H 1999 *Journal of Nuclear Materials* **274** 105.

[105] Cooper E A, Hughes C D, Earl W L and Sickafus K E 1995 *Materials Research Society Symposium Proceedings* **373** 413.

[106] Spence J C H and Taft J 1983 *Journal of Microscopy* **130** 147

[107] Soeda T, Matsumura S, Kinoshita C and Zaluzec N L 2000 *Journal of Nuclear Materials* **283** 952.

[108] Smith R, Bacorisen D, Uberuaga B P, Sickafus K E, Ball J A and Grimes R W 2005 *Journal of Physics: Condnsed Matter* **17** 875.

[109] Parker S C 1983 *Solid State Ionics* **8** 179.

[110] Cormack A N, Lewis G, Parker S C and Catlow C R A 1987 *Journal of Physics and Chemistry of Solids* **49** 53.

[111] Grimes R W, Anderson A B and Heuer A H 1989 *Journal of the American Ceramic Society* **111** 1.

[112] Wei S H and Zhang S B *Physical Review* **B63** 045112.

[113] Seko A, Yuge K, Oba F, Kuwabara A and Tanaka I 2006 *Physical Review B* **73** 184117.

[114] Kashii N, Maekawa H and Hinatsu Y 1999 *Journal of the American Ceramic Society* **82** 1844.

[115] Grimes N W, Thompson P and Kay H F 1983 *Proceedings of the Royal Society* **A386** 333.

[116] Baumgartner O, Preisinger A, Heger G and Guth H 1981 *Acta Crystallographica A* **37** C187.

[117] Andreozzi G B, Princivalle F, Skogby H and Giusta A D 2000 *American Mineralologist* **85** 1164.

[118] Docherty F T, Craven A J, McComb D W and Skakle J 2001 *Ultramicroscopy* **86** 273.

[119] Wood B J, Kirkpatrick R J and Montez B 1986 *American Mineralologist* **71** 999.

[120] Navrotsky A and Kleppa O J 1967 *Journal of Inorganic and Nuclear Chemistry* **29** 2701.

[121] M. Leslie, Technical Report, UK Science and Engineering Research Council - Daresbury Laboratory, Warrington (UK), 1982.

[122] Catlow C R A, Corish J, Jacobs P W M and Lidiard A B 1981 *Journal of Physics C: Solid State Physics* **14** 121.

[123] Vyas S, Grimes R W, Binks J D and Rey F 1997 *Journal of Physics and Chemistry of Solids* **58** 1619.

[124] Stoneham A M 1983 *Journal of Physics C: Solid State Physics* **16** L925.

[125] Nye J F 1985 *Physical Properties of Crystals* (Oxford: Oxford University Press)

[126] Chang Z P and Barsch G R 1973 *Journal of Geophysical Research* **78** 14.

[127] Lavrentiev M Y, Purton J A and Allan N L 2003 *American Mineralologist* **88** 1522.

[128] Gale J D 1997 *Journal of the Chemical Society Faraday Transactions* **93** 629.

[129] Segall M D, Lindan P J D, Probert M J, Pickard C J, Hasnip P J, Clark S J and Payne M C 2002 *Journal of Physics: Condensed Matter* **14** 2717.

[130] Perdew J P, Burke K and Ernzerhof M 1996 *Physics Review Letters* **77** 3865.

[131] Ceperley D M and Alder B J 1980 *Physics Review Letters* **45** 566.

[132] Perdew J P and Zunger A 1981 *Physics Review* **B23** 5048.

[133] Lagerlöf K P D and Grimes R W 1998 *Acta Materialia* **46** 5689.

[134] Kingery W D, Bowen H K and Uhlmann D R 1990, in *Introduction to Ceramics.* John Wiley, New York, 2nd edition.

[135] Broyden C G 1965 *Mathamatics of Computation* **19** 577.

[136] Chiang Y M and Kingery W D 1990 *Journal of the American Ceramic Society* **73** 841.

[137] Grimes N W 1972 *Philosophical Magazine* **25** 67.

[138] Ando K and Oishi Y 1974 *Journal of Chemical Physics* **63** 376.

[139] Ting C-J Lu H-Y 1999 *Journal of the American Ceramic Society* **82** 841.

[140] Uberuaga B P, Smith R, Cleave A R, Montalenti F, Henkelman G, Grimes R W, Voter A F, Sickafus K E 2004 *Physical Review of Letters* **92** 5505.

[141] Sørensen M R and Voter A F 2000 *Journal of Chemical Physics* **112** 9599.

[142] Voter A F, Montalenti F and Germann T C 2002 *Annual Review of Materials Research* **32** 321.

[143] Shannon R D 1976 *Acta Crystallographica* **32** 751.

[144] Bacrisen D *et al.*. in preparation.

[145] Ball J A, Grimes R W and Price D W 2005 *Modelling and Simulation in Materials Science and Engineering* **13** 1353.

[146] Greenwood N N 1968 *Ionic Crystals, Lattice Defects and Nonstoichiometry*, Butterworths.

[147] Wyckoff R W G 1963 *Crystal Structures*, volume 1. John Wiley & Sons 2nd edition.

[148] Islam M S and Balducci G 2002 in *Catalysis by Ceria and Related Materials*, Imperial College Press, London.

[149] Pryde A K A, Vyas S, Grimes R W, Gardner J A and Wang R P 1995 *Phisical Review* **B52** 13214.

[150] Balducci G, Kaspar J, Fornasiero P, Grazani M, Islam M S and Gale J D 1997 *Journal of Physical Chemistry* **B101** 1750.

[151] Adler S B, Smith J W and Reimer J A 1993 *Journal of the Chemical Society, Faraday Transactions* **98** 7613.

[152] Kilner J A and Waters C D 1982 *Solid State Ionics* **6** 253.

[153] Butler V, Catlow C R A, Fender B E F and Harding J H 1983 *Solid State Ionics* **8** 109.

[154] Kilner J A *Solid State Ionics* **8** 201.

[155] Murray A D, Murch G E and Catlow C R A 1986 *Solid State Ionics***18-19** 196.

[156] Meyer M, Nicoloso N and Jaenisch V 1997 *Physical Review* **B56** 5961.

[157] Zacate M O, Minervini L, Bradfield D J, Grimes R W and Sickafus K E 2000 *Solid State Ionics* **128** 243.

[158] Catlow C R A and Stoneham A M 1983 *Journal of Physics C: Solis State Physics* **16** 4321.

[159] Cong-Zhi B, Ji-Yun M, Jun Y, Xu F, Bai-Ru Z, Duan-Zheng Y and Xiang-Gang Q 2006 *Chinese Physics* **15** 1090.

[160] Xu Y-N and Ching W Y 1991 *Physical Review B* **43** 4461.