

References

- [1] V. P. Red'ko and L. M. Lopato. *Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy*, 27:1905–1910, 1991.
- [2] United Nations Framework Convention on Climate Change (UNFCCC). Report of the Conference of the Parties on its third session, held at Kyoto, from 1 to 11 December 1997. Technical Report FCCC/CP/1997/7, United Nations, 1998.
- [3] A. Cleave, R. W. Grimes, and K. Sickafus. *Phil. Mag.*, 85(9):967–980, 2005.
- [4] A. R. Cleave, R. W. Grimes, R. Smith, B. P. Uberuaga, and K. E. Sickafus. Simulations of cascades in pure and alumina doped magnesia: Implications for the Kinchin - Pease model. Awaiting publication in *Nucl. Instrum. Meth. B*, 2005.
- [5] F.A. Kroger. *The chemistry of imperfect crystals*, volume 2. North-Holland Publishing Company, Ltd., 2nd edition, 1974.
- [6] C. J. Dore, J. D. Watterson, J. W. L. Goodwin, T. P. Murrells, N. R. Passant, M. M. Hobson, S. L. Baggott, G. Thistlethwaite, P. J. Cole-

- man, K. R. King, M. Adams, and P. R. Cumine. UK emissions of air pollutants 1970 to 2002. Technical report, UK National Atmospheric Emissions Inventory (NAEI), October 2004.
- [7] G. W. Bush and M. Gorbachev. The Treaty Between The United States Of America And The Union Of Soviet Socialist Republics On The Reduction And Limitation Of Strategic Offensive Arms. Treaty, July 1991.
- [8] G. W. Bush and V. V. Putin. Treaty Between The United States Of America And The Russian Federation On Further Reduction And Limitation Of Strategic Offensive Arms (Start II). Treaty, January 1993.
- [9] G. W. Bush and V. V. Putin. Treaty between the united states of america and the russian federation on strategic offensive reductions. Treaty, May 2002.
- [10] P. Boczar, A. Dastur, K. Dormuth, A. Lee, and D. Meneley. *Prog. Nucl. Energ.*, 32(3/4):297–304, 1998.
- [11] H. W. Whittington. *Phil. Trans. R. Soc. Lond. A*, 360:1653–1668, 2002.
- [12] Department of Trade and Industry. Our energy future - creating a low carbon economy. White Paper Cm 5761, DTI, February 2003.
- [13] T. H. Hammons and H. K. Toh. *Electr. Pow. Compo. Sys.*, 29:277–295, 2001.

- [14] Nuclear power in the UK. Technical report, The Institution of Electrical Engineers, The Institution of Electrical Engineers, Savoy Place, London, February 2003.
- [15] P. D. Wilson, editor. *The Nuclear Fuel Cycle From Ore to Wastes*. Oxford University Press, Walton Street, Oxford, 1996.
- [16] H. Kleykamp. *J. Nucl. Mater.*, 131:221–246, 1985.
- [17] H. Kleykamp. *J. Nucl. Mater.*, 206:82–86, 1993.
- [18] R. W. Grimes and C. R. A. Catlow. *Phil. Trans. R. Soc. Lond. A*, 335:609–634, 1991.
- [19] S. Nicoll, H. J. Matzke, R. W. Grimes, and C. R. A. Catlow. *J. Nucl. Mater.*, 240:185–195, 1997.
- [20] J. T. Rogers, editor. *Fission Product Transport Processes in Reactor Accidents*. Hemisphere Publishing Corporation, 1990.
- [21] E. H. P. Cordfunke and R. J.M. Konings. *J. Nucl. Mater.*, 201:57–69, 1993.
- [22] S. T. Arm, R. P. Bush, and J. C. Mcgurk. *Prog. Nucl. Energ.*, 32:389–395, 1998.
- [23] Webster. Partitioning and transmutation of actinides and fission products consideration of medium and low level waste streams. In *Proceedings of the Third International Information Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation*. OECD Nuclear Energy Agency, 1994.

- [24] National report on compliance with the obligations of the joint convention on the safety of spent fuel management and on the safety of radioactive waste management. National report, Health and Safety Executive, 2003.
- [25] Managing the nuclear legacy - a strategy for action. Technical Report cm5552, Department for Trade and Industry, 2002.
- [26] W. J. Weber, R. C. Ewing, C. A. Angell, G. W. Arnold, A. N. Cormack, J. M. Delaye, D. L. Griscom, L. W. Hobbs, A. Navrotsky, D. L. Price, A. M. Stonham, and M. C. Weinberg. *J. Mat. Res.*, 12:1946–1978, 1997.
- [27] I. W. Donald, B. L. Metcalfe, and N.J. Taylor. *J. Mat. Sci.*, 32:5851–5887, 1997.
- [28] S. King. Management of plutonium: Disposal considerations. Technical Note 360756, Nirex, 2002.
- [29] L. A. Chick, G. F. Piepel, G. B. Mellinger, R. P. May, W. J. Gray, and L. Q. Buckwalter. The effects of composition on the properties in an 11 component nuclear-waste glass system. Technical Report PNL-3188, Pacific Northwest Laboratory, Battelle, 1981.
- [30] J. A. Fortner, A. J. Kropf, R. J. Finch, A. J. Bakel, M. C. Hash, and D. B. Chamberlain. *J. Nucl. Mater.*, 304(1):56–62, 2002.
- [31] R. C. Ewing, W. J. Weber, and J. Lian. *J. Applied Phys.*, 95(11):5949–5971, 2004.

- [32] K. Trachenko, M. T. Dove, and E. K. H. Salje. *Phys. Rev. B*, 65(18), 2002. Article No. 180102.
- [33] E. R. Vance, N. N. Watson, M. L. Carter, R. A. Day, and B. D. Begg. *J. Am. Ceram. Soc.*, 84(1):141–144, 2001.
- [34] K. B. Helean, A. Navrotsky, G. R. Lumpkin, M. Colella, J. Lian, R. C. Ewing, B. Ebbinghaus, and J. G. Catalano. *J. Nucl. Mater.*, 320:231–244, 2003.
- [35] S. X. Wang, B. D. Begg, L. M. Wang, R. C. Ewing, W. J. Weber, and K. V. G. Kutty. *J. Mater. Res.*, 12(12):4470–4473, 1999.
- [36] S. S. Shoup, C. E. Bamberger, and R. G. Haire. *J. Am. Ceram. Soc.*, 79(6):1489–1493, 1996.
- [37] H. Xu, Y. Wang, P. Zhao, W. L. Bourcier, R. Van Konynenburg, and H. Shaw. *Environ. Sci. Technol.*, 38:1480–1486, 2004. and references therein.
- [38] F. J. Dickson, K. D. Hawkins, and T. J. White. *J. Solid State Chem.*, 82:146–150, 1989.
- [39] A. E. Ringwood, S. E. Kesson, N. G. Ware, W. Hibberson, and A. Major. *Nature*, 278(5701):219–223, 1979.
- [40] A. E. Ringwood, S. E. Kesson, N. G. Ware, W. O. Hibberson, and A. Major. *Geochem. J.*, 13(4):141–165, 1979.

- [41] E. R. Vance, G. R. Lumpkin, M. L. Carter, D. J. Cassidy, C. J. Ball, R. A. Day, and B. D. Begg. *J. Am. Ceram. Soc.*, 85(7):1853–1859, 2002.
- [42] S. E. Kesson, W. J. Sinclair, and A. E. Ringwood. *Nucl. Chem. Waste Man.*, 4(3):259–265, 1983.
- [43] K. L. Smith, G. R. Lumpkin, M. G. Blackford, R. A. Day, and K. P. Hart. *J. Nucl. Mater.*, 190:287–294, 1992.
- [44] B. D. Begg, E. R. Vance, and G. R. Lumpkin. *Mat. Res. Symp. Proc.*, 506:79–86, 1998.
- [45] B. D. Begg, E. R. Vance, R. A. Day, M. Hambley, and S. D. Conradson. *Mat. Res. Symp. Proc.*, 465:325–340, 1997.
- [46] E. R. Vance, A. Jostsons, R. A. Day, B. D. Begg, , and P. J. Angel. *Mat. Res. Symp. Proc.*, 412:41–47, 1996.
- [47] E. R. Vance, P. J. Angel, B. D. Begg, and R. A. Day. *Mat. Res. Symp. Proc.*, 333:293–298, 1994.
- [48] E. R. Vance, B. D. Begg, R. A. Day, and C. J. Ball. *Mat. Res. Symp. Proc.*, 353:767–774, 1995.
- [49] A. Jostsons, E. R. Vance, D. J. Mercer, and V. M. Oversby. *Mat. Res. Symp. Proc.*, 353:775–781, 1995.
- [50] B. D. Begg, R. A. Day, and A. Brownscombe. *Mat. Res. Symp. Proc.*, 663:259–266, 2001.

- [51] R. L. Putnam, A. Navrotsky, B. F. Woodfield, J. Boerio-Goates, and J. L. Shapiro. *J. Chem. Thermodyn.*, 31(2):229–243, 1999.
- [52] B. F. Woodfield, J. Boerio-Goates, J. L. Shapiro, R. L. Putnam, and A. Navrotsky. *J. Chem. Thermodyn.*, 31(2):245–253, 1999.
- [53] R. Stevens, B. K. Hom, J. Boerio-Goates, B. F. Woodfield, R. L. Putnam, J. Gutierrez, and A. Navrotsky. *J. Chem. Thermodyn.*, 33(11):1441–1455, 2001.
- [54] R. L. Putnam, A. Navrotsky, B. F. Woodfield, J. L. Shapiro, R. Stevens, and J. Boerio-Goates. *Mat. Res. Soc. Symp. Proc.*, 556:11–18, 1999.
- [55] C. Meis, J. D. Gale, L. Boyer, J. Carpena, and D. Gosset. *J. Phys. Chem. A*, 104:5380–5387, 2000.
- [56] H. J. Matzke, E. Toscano, C. T. Walker, and A. G. Solomah. *Adv. Ceram. Mater.*, 3(3):285–288, 1988.
- [57] B. E. Burakov, E. E. Anderson, M. V. Zamoryanskaya, and M. A. Petrova. *Mat. Res. Soc. Symp. Proc.*, 608:419, 2000.
- [58] S. V. Yudinsev, S. V. Stefanovskii, O. I. Kir'yanova, J. Lian, and R. Ewing. *Atom. Energy*, 90(6), 2001.
- [59] S. Luo, L. Li, B. Tang, and D. Wang. *Waste Manage.*, 18:55–59, 1998.
- [60] D. R. Clarke. *Annu. Rev. Mater. Sci.*, 13:191–218, 1983.
- [61] W. J. Weber, R. C. Ewing., C. R. A. Catlow, T. D. de la Rubia, L. W. Hobbs, C. Kinoshita, H. Matzke, A. T. Motta, M. Nastasi, E. K. H.

- Salje, E. R. Vance, and S. J. Zinkle. Radiation effects in crystalline ceramics for the immobilization of high-level nuclear waste and plutonium. *J. Mater. Res.*, 13(6):1434–1484, 1998.
- [62] E. Fanchon, J. L. Hodeau, J. Vicat, and J. A. Watts. *J. Solid State Chem.*, 92:88–100, 1991.
- [63] H. J. Rossell. *J. Solid State Chem.*, 99:52–57, 1992.
- [64] A. R. Chakhmouradian and R. H. Mitchell. *J. Solid State Chem.*, 138:272–277, 1998.
- [65] F. W. Clinard, Jr., L. W. Hobbs, C. C. Land, D. E. Peterson, D. L. Rohr, and R. B. Roof. *J. Nucl. Mater.*, 105(2-3):248–256, 1982.
- [66] F. W. Clinard, Jr., D. E. Peterson, D. L. Rohr, and L. W. Hobbs. *J. Nucl. Mater.*, 126(3):245–254, 1984.
- [67] W. J. Weber, J. W. Wald, and H. J. Matzke. *J. Nucl. Mater.*, 138(2-3):196–209, 1986.
- [68] P. Martin, G. Carlot, A. Chevarie, C. Den-Auwer, and G. Panczer. *J. Nucl. Mater.*, 275:268–276, 1999.
- [69] W. J. Weber, R. C. Ewing, and A. Meldrum. *J. Nucl. Mater.*, 250(2-3):147–155, 1997.
- [70] A. Meldrum, L. A. Boatner, W. J. Weber, and R. C. Ewing. *Geochim. Cosmochim. Ac.*, 62(14):2509–2520, 1998.
- [71] R. C. Ewing. *P. Natl. A. Sci. USA.*, 96(7):3432–3439, 1999.

- [72] K. Trachenko, M. T. Dove, and E. K. H. Salje. *Phys. Rev. B*, 65(18), 2002.
- [73] K. Trachenko, M. T. Dove, and E. K. H. Salje. *J. Phys.-Cond. Matter.*, 15(2):L1–L7, 2003.
- [74] C. S. Palenik, L. Nasdala, and R. C. Ewing. *Am. Mineral.*, 88(5-6):770–781, 2003.
- [75] M. Zhang, E. K. H. Salje, and R. C. Ewing. *J. Phys.-Cond. Matter.*, 15(20):3445–3470, 2003.
- [76] T. Geisler, K. Trachenko, S. Rios, M. T. Dove, and E. K. H. Salje. *J. Phys.-Cond. Matter.*, 15(37):L597–L605, 2003.
- [77] R. C. Ewing, W. J. Weber, and F. W. Clinard. *Prog. Nucl. Energ.*, 150(1):209–212, 2000.
- [78] G. R. Lumpkin. *J. Nucl. Mater.*, 289(1-2):136–166, 2001.
- [79] J. F. DeNatale and D. G. Howitt. *Am. Ceram. Soc. Bull.*, 66:1393–1396, 1987.
- [80] W. J. Weber. *J. Minerals, Metals Mater. Soc.*, 43:35–39, 1991.
- [81] L. McFarland. Technical Report LALP 97-134, Los Alamos National Laboratory, Los Alamos, NM. U.S.A., November 1997 1997.
- [82] L. W. Hobbs and M. R. Pascucci. *J. Physique*, 41:237–241, 1980.
- [83] D. E. Beller, G. J. Van Tuyle, D. Bennett, G. Lawrence, K. Thomas, K. Pasamehmetoglu, N. Li, D. Hill, J. Laidler, and P. Fink. *Nucl.*

- Instrum. Methods Phys. Res., Sect. A, Accel. Spectrom.*, 463(3):468–486, 2001.
- [84] H. Nifenecker, S. David, J. M. Loiseaux, and O. Meplan. *Nucl. Instrum. Methods Phys. Res., Sect. A, Accel. Spectrom.*, 463(3):428–467, 2001.
- [85] M. Beauvy, T. Duverneix, C. Berlanga, R. Mazoyer, and C. Duriez. *J. Alloy. Compd.*, 271:557–562, 1998.
- [86] Asashi Kitamoto and Mulyanto. *Prog. Nucl. Energ.*, 32(3/4):429–437, 1997.
- [87] Mulyanto and A. Kitamoto. *Annals of Nuclear Energy*, 22(11):697–709, 1995.
- [88] R. C. Ewing and A. Macfarlane. *Science*, 296:659–660, April 2002.
- [89] N. Morner. *Eng. Geol.*, 61(2-3):75–82, 2001.
- [90] A. M. Beauchesne and J. Boese. Technical report, National Governors Association Center for Best Practices, National Governors Association, 444 North Capitol Street, Washington, D.C., 2000.
- [91] Accelerating cleanup - paths to closure. Technical Report DOE/EM-0362, U.S. Department of Energy (DOE), U.S. Department of Energy (DOE) Office of Environmental Management, Washington, DC., June 1998.
- [92] M. Holt. Civilian nuclear waste disposal. Technical Report IB92059, The National Council for Science and the Environment, April 2001.

- [93] J. E. Mielke. Proposed high-level nuclear waste repository: Yucca mountain site characterization progress. Report for Congress RL30190, The Committee for the National Institute for the Environment, May 1999.
- [94] Scientific and technical basis for geological disposal of radioactive wastes. Technical Report STI/DOC/010/413, International Atomic Energy Agency, Vienna, 2003.
- [95] A. Hedin. Technical Report 9713, Swedish Nuclear Fuel and Waste Management Co, 1997.
- [96] L. L. Hench, D. E. Clark, and A. B. Harker. *J. Mater. Sci.*, 21:1457–1478, 1986.
- [97] P. Toulhoat. Confinement and migration of radionuclides in a nuclear waste deep repository. In Press *C. R. Physique 0* (2002) 112.
- [98] S. Stewart. *Eng. Geol.*, 67(1-2):139–168, 2002.
- [99] M. Born. *Atomtheorie des Festen Zustandes*. Teubner, Leipzig, 1923.
- [100] P. P. Ewald. *Ann. der Physik*, 65:253, 1921.
- [101] C. Kittel. *Introduction to Solid State Physics*. John Wiley & Sons, New York, 1st printing edition, 1953.
- [102] M. Leslie. DI/sci/tm31t. Technical report, SERC Daresbury Laboratory, 1982.
- [103] J. D. Gale. *J. Chem. Soc. Faraday T.*, 93(4):629–637, 1997.

- [104] W. Pauli. *Z. Physik*, 31:765, 1925.
- [105] F. London. *Z. Physik*, 63:245, 1930.
- [106] F. London. *Z. Physik Chem.*, 11:222, 1930.
- [107] R. Eisenschitz and F. London. *Z. Physik*, 60:491, 1930.
- [108] M. Born and A. Landé. *Verhandlungen der Deutschen Physik Gesellschaft*, 21/24:210, 1918.
- [109] M. Born and J.E. Mayer. *Z. Physik*, 75:1, 1932.
- [110] J. E. Lennard-Jones. *Proc. R. Soc. Lon. A*, page 463, 1924.
- [111] R. A. Buckingham. *Proc. Royal Soc. London. Series A, Math. Phys. Sci.*, 168:264–283, 1938.
- [112] L. Minervini, R. W. Grimes, Y. Tabira, R. L. Withers, and K. E. Sickafus. *Phil. Mag. A*, 82:123–135, 2002.
- [113] B. G. Dick and A. W. Overhauser. *Phys. Rev.*, 112:90–112, 1958.
- [114] C. R. A. Catlow and W. C. Mackrodt. Theory of simulation methods for lattice and defect energy calculations in crystals. In C. R. A. Catlow and W. C. Mackrodt, editors, *Computer Simulation of Solids*, Berlin, 1982. Springer-Verlag.
- [115] U. Schroder. *Solid State Commun.*, 4(7):347–349, 1966.
- [116] M. J. L. Sangster. *J. Phys. Chem. Solids*, 35:195–200, 1974.
- [117] N. F. Mott and M. J. Littleton. *Trans. Faraday Soc.*, 34:485, 1932.

- [118] J. F. Ziegler, J. P. Biersack, and U. Littmark. *The Stopping and Range of Ions in Solids*, volume 1. Pergamon, Oxford, 1985.
- [119] R. Smith, D. Bacorisen, B. P. Uberuaga, K. E. Sickafus, J. A. Ball, and R. W. Grimes. *J. Phys.-Cond. Matter.*, 17(6):875=891, 2005.
- [120] W. T. Rankin and J. A. Board Jr. A portable distributed implementation of the parallel multipole tree algorithm. In *Fourth IEEE International Symposium on High Performance Distributed Computing (HPDC-4 '95)*, page 17, Los Alamitos, CA, 1995. IEEE Comput. Soc. Press.
- [121] L. Greengard. *The Rapid Evaluation of Potential Fields in Particle Systems*. MIT Press, Cambridge, MA, 1988.
- [122] R. D. Adamson. *Novel Methods for Large Molecules in Quantum Chemistry*. Phd thesis, University of Cambridge, Trinity College, Cambridge, January 1999.
- [123] L. Verlet. *Phys. Rev.*, 159(1):98–103, 1967.
- [124] M. J. Norgett. A general formulation of the problem of calculating the energies of lattice defects in ionic crystals. Technical Report R.7650 HL74/335, Atomic Energy Research Establishment, Harwell, 1974.
- [125] R. Smith. *Atom and Ion Collisions in Solids and at Surfaces*. Cambridge University Press, Cambridge, 1997.
- [126] Hj. Matzke. *Nucl. Instrum. Meth. B*, 65:30–39, 1992.

- [127] K. E. Sickafus, Hj. Matzke, Th. Hartmann, K. Yasuda, J. A. Valdez, P. Chodak III, M. Nastasi, and R. A. Verrall. *J. Nucl. Mater.*, 274(1-2):66–77, 1999.
- [128] N. Yu, K. E. Sickafus, P. Kodali, and M. Nastasi. *J. Nucl. Mater.*, 244(3):266–272, 1997.
- [129] K. Yasuda, M. Nastasi, K. E. Sickafus, C. J. Maggiore, and N. Yu. *Nucl. Instrum. Meth. B*, 136-138:499–504, 1998.
- [130] K. E. Sickafus, J. A. Valdez, J. R. Williams, R. W. Grimes, and H. T. Hawkins. *Nucl. Instrum. Meth. B*, 191(1-4):549–558, 2002.
- [131] K. E. Sickafus, L. Minervini, R. W. Grimes, J. A. Valdez, and T. Hartmann. *Radiat. Eff. Defect. S.*, 155(1-4):133–137, 2001.
- [132] K. E. Sickafus, L. Minervini, R. W. Grimes, J. A. Valdez, M. Ishimaru, F. Li, K. J. McClellan, and T. Hartmann. *Science*, 289(5480):748–751, 2000.
- [133] C. Degueldre and C. Hellwig. *J. Nucl. Mater.*, 320(1-2):96–105, 2003.
- [134] K.E. Sickafus, R.J. Hanrahan, K.J. McClellan, J.N. Mitchell, C.J. Wetland, D.P. Butt, P. Chodak, K.B. Ramsey, T.H. Blair, K. Chidester, Hj. Matzke, K. Yasuda, R.A. Verrall, and N. Yu. *Am. Ceram. Soc. Bull.*, 78(1):69–74, 1999.
- [135] M. A. Subramanian, G. Aravamudan, and G. V. Subba Rao. *Prog. Solid St. Chem*, 15:55–143, 1983.

- [136] J. Wang, Y. Xie, Z. Zhang, R. Liu, and Z. Li. *Mater. Res. Bull.*, 40(8):1294–1302, 2005.
- [137] Y. Shimizu and K. Maeda. *Sensor. Actuat. B-Chem.*, 52(1-2):84–89, 1998.
- [138] Tetsuo Shimura, Masakage Komori, and Hiroyasu Iwahara. *Solid State Ionics*, 86-88(Part 1):685–689, 1996.
- [139] A. Weyl and D. Janke. *J. Am. Ceram. Soc.*, 79(8):2145–2155, 1996.
- [140] O. Porat, M. A. Spears, C. Heremans, I. Kosacki, and H. L. Tuller. *Solid State Ionics*, 86-8:285–288, 1996. Part 1.
- [141] J. T. S. Irvine S. Tao. *The Chemical Record*, 4(2):83–95, 2004.
- [142] O. Porat, C. Heremans, and H. L. Tuller. *Solid State Ionics*, 94(1-4):75–83, 1997.
- [143] O. Porat, C. Heremans, and H. L. Tuller. *J. Am. Ceram. Soc.*, 80(9):2278–2284, 1997.
- [144] J. J. Sprague and H. L. Tuller. *J. Eur. Ceram. Soc.*, 19(6-7):803–806, 1999.
- [145] T. Takeda, R. Kanno, Y. Kawamoto, Y. Takeda, and O. Yamamoto. *J. Electrochem. Soc.*, 147(5):1730–1733, 2000.
- [146] T. Takeda, R. Kanno, K. Tsubosaka, and Y. Takeda. *Electrochemistry*, 70(12):969–971, 2002.
- [147] J. M. Bae and B. C. H. Steele. *J. Electroceram.*, 3(1):37–46, 1999.

- [148] J. H. Ke, A. S. Kumar, J. W. Sue, S. Venkatesan, and J. M. Zen. *J. Mol. Catal. A-Chem.*, 233(1-2):111–120, 2005.
- [149] J. M. Zen, A. S. Kumar, and H. P. Chen. *Electroanal.*, 15(20):1584–1588, 2003.
- [150] J. M. Sohn, M. R. Kim, and S. I. Woo. *Catal. Today*, 83(1-4):289–297, 2003.
- [151] H. Wang, H. L. Du, Z. Peng, M. L. Zhang, and X. Yao. *Ceram. Int.*, 30(7):1225–1229, 2004.
- [152] H. L. Du, H. Wang, and X. Yao. *Ceram. Int.*, 30(7):1383–1387, 2004.
- [153] G. K. Choi, D. W. Kim, S. Y. Cho, and K. S. Hong. *Ceram. Int.*, 30(7):1187–1190, 2004. Sp. Iss. SI.
- [154] A. Dimoulas, G. Vellianitis, G. Mavrou, G. Apostolopoulos, A. Travlos, C. Wiemer, M. Fanciulli, and Z. M. Rittersma. *Appl. Phys. Lett.*, 85(15):3205–3207, 2004.
- [155] C. Ang and Z. Yu. *Phys. Rev. B*, 70(13), 2004.
- [156] N. Nadaud, N. Lequeux, M. Nanot, J. Jové, and T. Roisnel. *J. Solid State Chem.*, 135:140–148, 1998.
- [157] A. Bogicevic and C. Wolverton. *Phys. Rev. B*, 67:024106, 2003.
- [158] A. Bogicevic, C. Wolverton, G. M. Crosbie, and E. B. Stechel. *Phys. Rev. B*, 64:014106, 2001.

- [159] M. Chen, B. Hallstedt, and L. J. Gaukler. *Solid State Ionics*, 170:255–274, 2004.
- [160] L. M. Lopato, V. P. Red'ko, G. I. Gerasimiyuk, and A. V. Shevchenko. *Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy*, 27:1718–1722, 1991.
- [161] M. R. Thornber, D. J. M. Bevan, and J. Graham. *Acta Cryst. B*, 24:1183–1190, 1968.
- [162] B.J. Kennedy, B.A. Hunter, and C.J. Howard. *J. Solid State Chem.*, 130:58–65, 1997.
- [163] N. F. M. Henry and K. Lonsdale, editors. *International Tables for X-ray Crystallography*, volume 1. The Kynoch Press, Birmingham, 1952.
- [164] C.K. Jorgensen and E. Rittershaus. *Kongelige Danske Videnskabernes Selskab, Matematisk-Fysike Meddelelser*, 35:1–37, 1967.
- [165] M. Glerup, O. F. Nielsen, and F. W. Poulsen. *J. Solid State Chem.*, 160:25–32, 2001.
- [166] H.W. Schmalle, T. Williams, A. Reller, A. Linden, and J.G. Bednorz. *Acta Cryst. B*, 49:235–244, 1993.
- [167] P. Duran and C. Pascual. *J. Mater. Sci.*, 19:1178–1184, 1984.
- [168] A. V. Zagorodnyuk, L. V. Sadkovskaya, G. V. Shamrai, I.P. Kovalenskaya, R. L. Magunov, and G. A. Teterin. *Russ. J. Inorg. Chem.*, 31:1377, 1986.

- [169] G. V. Shamrai, R. L. Magunov, I. V. Stasenko, and A. P. Zhirnova. *Inorg. Chem.*, 25:233, 1989.
- [170] A.V. Zagorodnyuk G.A. Teterin, V.F. Zinchenko and I.M. *Sov. Progr. Chem.*, 54:31, 1988.
- [171] N. Mizutani, Y. Tajima, and M. Kato. *J. Am. Ceram. Soc.*, 59:168, 1976.
- [172] G. V. Shamrai, R. L. Magunov, and I. P. Kovalevskaya. *Inorg. Mater.*, 22:1695, 1986.
- [173] A. V. Kolesnikov, G. E. Sukhanova, A. P. Zaitseva, and L. G. Scherbakova. *Inorg. Mater.*, 23:222, 1987.
- [174] R. D. Shannon. *Acta Cryst.*, 32:751–767, 1976.
- [175] A. V. Shevchenko, L. M. Lopato, and I. E. Kiryakova. *Inorg. Mater.*, 20:1731, 1984.
- [176] A. V. Shevchenko and L. M. Lopato. *Inorg. Mater.*, 18:1583, 1982.
- [177] L. M. Lopato A. V. Shevchenko and L. V. Nazarenko. *Inorg. Mater.*, 20:1615, 1984.
- [178] L. M. Lopato A. V. Shevchenko and Z. A. Zaitseva. *Inorg. Mater.*, 20:1316, 1984.
- [179] S. S. Kiparisov, R. A. Belyaev, A. I. Belyakov, V. V. Kondarenko, V. P. Vyskubov, V. G. Kozlov, S. A. Kuznetsov, and L. P. Melikhova. *Inorg. Mater.*, 12:1393, 1976.

- [180] M. P. y Jorba. *Ann. Chim. (Paris)*, 7:479, 1962.
- [181] A. Rouanet. *Rev. Int. Hautes Temp. Refract.*, 8:161, 1971.
- [182] F. H. Brown Jr. and P. Duwez. *J. Am. Ceram. Soc.*, 38:95, 1955.
- [183] R. S. Roth. *J. Res. Natl. Bur. Std.*, 56:24, 1956.
- [184] H. Yokokawa, N. Sakai, T. Horita, K. Yamaji, T. Otake, H. Yugami, T. Kawada, and J. Mizusaki. *J. Phase Equilib.*, 22:331, 2001.
- [185] V. S. Stubican, R. C. Hink, and S. P. Ray. *J. Am. Ceram. Soc.*, 61:17, 1978.
- [186] P. S. Duwez and F. H. Brown Jr. *J. Electrochem. Soc.*, 98:360, 1951.
- [187] K. K. Srivastava, R. N. Patil, C. B. Choudhary, K. V. G. K. Gokhale, and E. C. Subbarao. *Trans. J. Br. Ceram. Soc.*, 73:85, 1974.
- [188] H.G. Scott. *J. Mater. Sci.*, 10:1527, 1975.
- [189] H.G. Scott. *J. Aust. Ceram. Soc.*, 17:16, 1982.
- [190] V. S. Stubican and J. R. Hellmann. *Adv. Ceram.*, 3:25, 1981.
- [191] FIZ Karlsruhe Information Services. Inorganic crystal structure database. <http://icsdweb.fiz-karlsruhe.de/>, 2005.
- [192] A. W. Sleight. *Inorg. Chem*, 8(8):1807–1808, 1969.
- [193] O. Knop, F. Brisse, L. Castelliz, and R. Sutarno. *Can. J. Chem.*, 43:2812–2826, 1965.
- [194] F. Brisse and O. Knop. *Can. J. Chem.*, 46:859–873, 1968.

- [195] O. Knop, F. Brisse, and L. Castelliz. *Can. J. Chem.*, 47:971–990, 1969.
- [196] H.-J. Deiseroth and H. Mueller-Buschbaum. *Z. Anorg. Allg. Chem.*, 375:152–156, 1970.
- [197] M. Faucher and P. Caro. *J. Solid State Chem.*, 12:1–11, 1975.
- [198] M.P. van Dijk, J.H.H. Ter Maat, G. Roelofs, H. Bosch, G.M.H. van de Velde, P.J. Gellings, and A.J. Burggraaf. *Mater. Res. Bull.*, 19:1149–1156, 1984.
- [199] G.M.H. van de Velde, B.C. Lippens, S.J. Korf, and J. Boeijmsma. *Powder Diffr.*, 5:229–231, 1990.
- [200] T. Yamamoto, R. Kanno, Y. Takeda, O. Yamamoto, Y. Kawamoto, and M. Takano. *J. Solid State Chem.*, 109:372–383, 1994.
- [201] H. Kobayashi, R. Kanno, Y. Kawamoto, T. Kamiyama, F. Izumi, and A.W. Sleight. *J. Solid State Chem.*, 114:15–23, 1995.
- [202] B.J. Kennedy. *Mater. Sci. Forum*, 228:753–758, 1996.
- [203] B.J. Kennedy and T. Vogt. *J. Solid State Chem.*, 126:261–270, 1996.
- [204] E. Chtoun, L. Hanebali, P. Garnier, and J.-M. Kiat. *Eur. J. Solid State Inorg. Chem.*, 34:553–561, 1997.
- [205] B.J. Kennedy, B.A. Hunter, and C.J. Howard. *J. Solid State Chem.*, 130:58–65, 1997.
- [206] M. Field, B.J. Kennedy, and B.A. Hunter. *J. Solid State Chem.*, 151:25–30, 2000.

- [207] E. Chtoun, L. Hanebali, and P. Garnier. *Ann. Chim.*, 26:27–32, 2001.
- [208] Y. Tabira, R.L. Withers, T. Yamada, and N. Ishizawa. *Z. Kristallogr.*, 216:92–98, 2001.
- [209] C. Bansal, H. Kawanaka, H. Bando, and Y. Nishihara. *Phys. Rev., Serie 3. B - Condensed Matter*, 66:052406–1–052406–4, 2002.
- [210] N. Taira, M. Wakeshima, Y. Hinatsu, A. Tobo, and K. Ohoyama. *J. Solid State Chem.*, 176:165–169, 2003.
- [211] Y. Moritomo, Sh. Xu, A. Machida, T. Katsufuji, E. Nishibori, M. Takata, M. Sakata, and S-W. Cheong. *Phys. Rev. B*, 63:144425, 2001.
- [212] L.M. Red'ko, V.P.;Lopato. *Dopov. Akad. Nauk. A*, 1990:78–81, 1990.
- [213] H.J. Rossell. *J. Solid State Chem.*, 19:103–111, 1976.
- [214] M.R. Thornber and D.J.M. Bevan. *J. Solid State Chem.*, 1:536–544, 1970.
- [215] G. Brauer and H. Gradinger. *Zeitschrift fuer Anorganische und Allgemeine Chemie*, 276:209–226, 1954.
- [216] A. Rabenau. *Zeitschrift fuer Anorganische und Allgemeine Chemie*, 288:221–234, 1956.
- [217] C.K. Jorgensen and E. Rittershaus. *Kongelige Danske Videnskabernes Selskab, Matematisk-Fysike Meddelelser*, 35:1–37, 1967.

- [218] T. Moriga, A. Yoshiasa, F. Kanamaru, K. Koto, M. Yoshimura, and S. Somiya. *Solid State Ionics*, 31:319–328, 1989.
- [219] B. J. Wuensch, K. W. Eberman, C. Heremans, E. M. Ku, P. Onnerud, E. M. E. Yeo, S. M. Haile, J. K. Stalick, and J. D. Jorgensen. *Solid State Ionics*, 129(1-4):111–133, 2000.
- [220] C. R. Stanek, L. Minervini, and R.W. Grimes. *J. Am. Ceram. Soc.*, 85(11):2792–2798, 2002.
- [221] M. Pirzada, R. W. Grimes, L. Minervini, J. F. Maguire, and K. E. Sickafus. *Solid State Ionics*, 140:201–208, 2001.
- [222] M. P. van Dijk, A. J. Burggraaf, A. N. Cormack, and C. R. A. Catlow. *Solid State Ionics*, 17(2):159–167, 1985.
- [223] L. Minervini, R. W. Grimes, and K. E. Sickafus. *J. Am. Ceram. Soc.*, 83:1873–78, 2000.
- [224] W. R. Panero, L. P. Stixrude, and R. C. Ewing. *Phys. Rev. B.*, 70(5):054110, 2004.
- [225] C. R. Stanek and R. W. Grimes. *J. Am. Ceram. Soc.*, 85(8):2139–2141, 2002.
- [226] M. J. D. Rushton, R. W. Grimes, C. R. Stanek, and S. Owens. *J. Mater. Res.*, 19(6):1603–1604, 2004.
- [227] P. J. Wilde and C. R. A. Catlow. *Solid State Ionics*, 112(3-4):173–183, 1998.

- [228] P. J. Wilde and C. R. A. Catlow. *Solid State Ionics*, 112(3-4):185–195, 1998.
- [229] G. Kresse and J. Hafner. *Phys. Rev. B*, 47:558, 1993.
- [230] C. R. Stanek and R. W. Grimes. *J. Am. Ceram. Soc.*, 85:2139–2141, 2002.
- [231] K. E. Sickafus and J. Valdez. Private Communication, 2005.
- [232] K. E. Sickafus, L. Minervini, R. W. Grimes, J. E. Valdez, and T. Hartmann. *Rad. Eff. Defects Solids*, 155:133–137, 2001.
- [233] J. Lian, X. T. Zu, K. V. G. Kutty, J. Chen, L. M. Wang, and R. C. Ewing. *Phys. Rev. B*, 66(5), 2002.
- [234] R. E. Williford and W. J. Weber. Computer simulation of Pu^{3+} and Pu^{4+} substitutions in gadolinium zirconate. *J. Nucl. Mater.*, 299(2):140–147, 2001.
- [235] J. Lian, L. M. Wang, G. R. Lumpkin, and R. C. Ewing. *Nucl. Instrum. Methods Phys. Res. Sect. B: Beam Interact. Mater.*, 191:565–570, 2002.
- [236] W. L. Gong, W. Lutze, and R. C. Ewing. *J. Nucl. Mater.*, 277:239–249, 2000.
- [237] A. R. Boccaccini, S. Atiq, and R. W. Grimes. *Adv. Eng. Mater.*, 5(7):501–508, 2003.
- [238] H. Xu and Y. Wang. *J. Nucl. Mater.*, 275:216–220, 1999.

- [239] K. B. Helean, A. Navrotsky, E. R. Vance, M. L. Carter, B. Ebbinghaus, O. Krikorian, J. Lian, L. M. Wang, and J. G. Catalano. *J. Nucl. Mater.*, 303:226–239, 2002.
- [240] S. Yamazaki, T. Yamashita, T. Matsui, and T. Nagasaki. *J. Nucl. Mater.*, 294:183–187, 2001.
- [241] I. Hayakawa and H. Kamizono. *J. Nucl. Mater.*, 202:163–168, 1993.
- [242] N. K. Kulkarni, S. Sampath, and V. Venugopal. *J. Nucl. Mater.*, 281:248–250, 2000.
- [243] H. Yokoi, Y. Arita, T. Matsui, H. Ohno, and K. Kobayashi. *J. Nucl. Mater.*, 238:163–168, 1996.
- [244] Laurence A. J. Garvie, Huifang Xu, Yifeng Wang, and Robert L. Putnam. *J. Phys. Chem. Solids*, 66:902–905, 2005.
- [245] E. R. Vance, M. L. Carter, M. W. A. Stewart, R. A. Day, B. D. Begg, and C. J. Ball. *Mat. Res. Soc. Symp. Proc.*, 713:319–326, 2002.
- [246] S. X. Wang, L. M. Wang, R. C. Ewing, and K. V. Govindan Kutty. *Nucl. Instrum. Meth. B*, 169:135–140, 2000.
- [247] J. Lian, L. Wang, J. Chen, K. Sun, R. C. Ewing, J. Matt Farmer, and L. A. Boatner. *Acta Mater.*, 51:1493–1502, 2003.
- [248] B. C. Chakoumakos. *J. Solid State Chem.*, 53(1):120–129, 1984.
- [249] D. D. Hogarth, C. T. Williams, and P. Jones. *Mineral. Mag.*, 64(4):683–697, 2000.

- [250] R. E. Sykora, P. E. Raison, and R. G. Haire. *J. Solid State Chem.*, 178(2):578–583, 2005. Sp. Iss. SI.
- [251] M. J. Apted, D. Langmuir, D. W. Moeller, J. A., A. E. Waltar, D. von Winterfeldt, R. C. Ewing, and A. Macfarlane. *Science*, pages 2333–2335, 2002.
- [252] D. M. Strachan, R. D. Scheele, E. C. Buck, J. P. Icenhower, A. E. Kozelisky, R. L. Sell, R. J. Elovich, and W. C. Buchmiller. *J. Nucl. Mater.*, 345(2-3):109–135, 2005.
- [253] D. M. Strachan, R. D. Scheele, W. C. Buchmiller, J. D. Vienna, R. L. Sell, and R. J. Elovich. Preparation and characterization of 238 Pu-ceramics for radiation damage experiments. Technical Report PNNL-13251, Pacific Northwest Laboratory, Richland, Washington 99352, May 2000.
- [254] D. M. Strachan, R. D. Scheele, J. P. Icenhower, A. E. Kozelisky, R. L. Sell, V. L. Legore, H. T. Schaefer, M. J. OHara, C. F. Brown, and W. C. Buchmiller. The status of radiation damage experiments. Technical Report PNNL-13721, Pacific Northwest Laboratory, Richland, Washington 99352, November 2001.
- [255] G. R. Lumpkin, K. R. Whittle, S. Rios, K. L. Smith, and N. J. Zaluzec. *J. Phys.-Cond. Matter.*, 16(47):8557–8570, 2004.
- [256] J. Lian, R. C. Ewing, L. M. Wang, and K. B. Helean. *J. Mater. Res.*, 19(5):1575–1580, 2004.

- [257] J. Lian, L. M. Wang, R. G. Haire, K. B. Helean, and R. C. Ewing. *Nucl. Instrum. Meth. B*, 218:236–243, 2004.
- [258] Y. Zhang, W. J. Weber, V. Shutthanandan, R. Devanathan, S. Thevuthasan, G. Balakrishnan, and D. M. Paul. *J. Appl. Phys.*, 95(5):2866–2872, 2004.
- [259] J. Lian, J. Chen, L. M. Wang, R. C. Ewing, J. M. Farmer, L. A. Boatner, and K. B. Helean. *Phys. Rev. B*, 68(13), 2003.
- [260] B. D. Begg, N. J. Hess, W. J. Weber, R. Devanathan, J. P. Icenhower, S. Thevuthasan, and B. P. McGrail. *J. Nucl. Mater.*, 288(2-3):208–216, 2001.
- [261] G. R. Lumpkin, K. L. Smith, and M. G. Blackford. *J. Nucl. Mater.*, 289(1-2):177–187, 2001.
- [262] A. Meldrum, C. W. White, V. Keppens, L. A. Boatner, and R. C. Ewing. *Phys. Rev. B*, 6310(10), 2001.
- [263] S. X. Wang, L. M. Wang, R. C. Ewing, G. S. Was, and G. R. Lumpkin. *Nucl. Instrum. Meth. B*, 148(1-4):704–709, 1999.
- [264] J. A. Purton and N. L. Allan. *J. Mater. Chem.*, 12(10):2923–2926, 2002.
- [265] A. Chartier, C. Meis, J. P. Crocombette, L. R. Corrales, and W. J. Weber. *Phys. Rev. B*, 67(17), 2003.
- [266] A. Chartier, C. Meis, J. P. Crocombette, W. J. Weber, and L. R. Corrales. *Phys. Rev. Lett.*, 94(2), 2005.

- [267] G. Busker, A. Chroneos, and R. W. Grimes. *J. Am. Ceram. Soc.*, 82:1553–1559, 1999.
- [268] V. Butler, C. R. A. Catlow, and B. E. F. Fender. *Radit. Eff.*, 73:273, 1983.
- [269] R.E. Williford, W.J. Weber, R. Devanathan, and J.D. Gale. *J. Electroceram.*, 3:409–424, 1999.
- [270] N. L. Allan, G. D. Barrera, T. H. K. Barron, and M. B. Taylor. *Int. J. Thermophysics*, 22(2):535–546, 2001.
- [271] M. Samaras, P. M. Derlet, H. Van Swygenhoven, and M. Victoria. *Phil. Mag.*, 83(31-34):3599–3607, 2003.
- [272] M. J. Giacobbe, N. Q. Lam, L. E. Rehn, P. M. Baldo, L. Funk, and J. F. Stubbins. *J. Nucl. Mater.*, 281(2-3):213–224, 2000.
- [273] F. J. Perez-Perez and R. Smith. *Nucl. Instrum. Meth. B*, 164:487–494, 2000.
- [274] S. J. Zinkle and C. Kinoshita. *J. Nucl. Mater.*, 251:200–217, 1997.
- [275] R. H. Jones, D. Steiner, H. L. Heinisch, G. A. Newsome, and H. M. Kerch. *J. Nucl. Mater.*, 245(2-3):87–107, 1997.
- [276] T. D. delaRubia, J. M. Perlado, and M. Tobin. *J. Nucl. Mater.*, 237:1096–1101, 1996. Part B.
- [277] S. Vyas, R. W. Grimes, D. J. Binks, and F. Rey. *J. Phys. Chem. Solids*, 58(10):1619–1624, 1997.

- [278] C. Kinoshita, K. Hayashi, and S. Kitajima. *Nucl. Instrum. Meth. B*, 229(2-3):209–218, 1984.
- [279] G. H. Kinchen and R. S Pease. *Rep. Prog. Phys.*, 18:1, 1955.
- [280] M. J. Norgett and M. T. Robinson. *Nucl.Eng.Des.*, 33:50, 1975.
- [281] D. J. Bacon, F. Gao, and Yu. N. Osetsky. *Nucl. Instrum. Meth. B*, 153(1-4):87–98, June 1999.
- [282] J. Gittus. *Irradiation Effects in Crystalline Solids*. Applied Science Publishers Ltd, London, 1978.
- [283] S. J. Zinkle and B. N. Singh. *J. Nucl. Mater.*, 199:173–191, 1993.
- [284] H. Huang and N. Ghoniem. *J. Nucl. Mater.*, 199:221–230, 1993.
- [285] B. P. Uberuaga, R. Smith, A. R. Cleave, G. Henkelman, R. W. Grimes, A. F. Voter, and K. E. Sickafus. *Phys. Rev. B*, 71(10):104102, 2005.
- [286] R. E. Williford, R. Devanathan, and W. J. Weber. *Nucl. Instrum. Meth. B*, 141(1-4):94–98, 1998.
- [287] B. Park, W. J. Weber, and L. R. Corrales. *Nucl. Instrum. Meth. B*, 166-167:357–363, 2000.
- [288] C. Y. Tang, X. Yao, J. Hu, Q. L. Rao, Y. R. Li, and B. W. Tao. *Supercond. Sci. Tech.*, 18(6):L31–L34, 2005.
- [289] Watlow Electric. Smart technology to heat up the foodservice industry. Report, Watlow Electric Manufacturing Company, 2000.
- [290] R. W. Grimes. *J. Am. Ceram. Soc*, 77(2):378–384, 1994.

- [291] C. R. A. Catlow, I. D. Faux, and M. J. Norgett. *J. Phys. C: Solid State Phys.*, 9:419–429, 1976.
- [292] A. Aguado and P. A. Madden. *Phys. Rev. Lett.*, 94(6), 2005.
- [293] G. Busker, M. A. van Huis, R. W. Grimes, and A. van Veen. *Nucl. Instrum. Meth. B*, 171(4):528–536, 2000.
- [294] V.G. Tsirel'son, A.S. Avilov, Yu.A. Abramov, E.L. Belokoneva, R. Kitaneh, and D. Feil. *Acta Cryst. B*, 54:8–17, 1998.
- [295] E. Alves, R. C. da Silva, J.V. Pinto, T. Monteiro, B. Savoini, D. Cáceres, R. González, and Y. Chen. *Nucl. Instrum. Meth. B*, 206:148–152, 2003.
- [296] R. González, I. Vergara, D. Cáceres, and Y. Chen. *Phys. Rev. B*, 65:224108, 2002.
- [297] W. A. Sibley and Y. Chen. *Phys. Rev.*, 160(3):412–716, 1967.
- [298] B. Henderson, D. H. Bowen, A. Briggs, and R. D. King. *J. Phys. C: Solid State*, 4(12):1496–1504, 1971.
- [299] B. P. Uberuaga, R. Smith, A. R. Cleave, F. Montalenti, G. Henkelman, R. W. Grimes, A. F. Voter, and K. E. Sickafus. *Phys. Rev. Lett.*, 92(11):115505, 2004.
- [300] J. F. Ziegler, J. P. Bierrack, and U. Littmark. *The Stopping and Range of Ions*, volume Volume 1. Pergamon, Oxford, 1985.
- [301] M.I. McCarthy and N.M. Harrison. *Phys. Rev. B*, 49:8574–8582, 1994.

[302] D. Taylor. *Brit. Ceram. Trans. Soc.*, 83:5–9, 1984.

[303] K. Hirata, K. Moriya, and Y. Waseda. *J. Mater. Sci.*, 83:5–9, 1977.