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Stresses in Local Volumes During Reactive Sintering of Powder Mixture Ti-Al-Fe-Fe_2O_3

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Abstract. Composites based on titanium and aluminium have been attracting attention for decades. One of the possible ways of creating such composites is based on reaction sintering, which implies sintering with accompanying chemical reactions, the consequence of which is a change in phase composition. The number of reactions may directly include those that lead to the formation of the hardening phase. Mixtures of the Ti-Al-Fe-Fe_2O_3 type, where the source of iron oxide is metalworking waste, are very promising for use in this direction. However, for multicomponent systems the regularities of phase formation, as well as the appearance of stresses in the diffusion zone, are not obvious and are not the same for the entire volume of reaction mixtures. The present paper describes general ideas and methods of modelling for reactive sintering and gives an overview of the situations that are most important for phase formation in a selected mixture. It is shown that the dynamics of phase growth and stresses can be different in different local volumes with various variants of particles meeting each other.

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REFERENCES

[1] E.N. Korosteleva, A.G. Knyazeva, I.O. Nikolaev, Phase Formation in Reactive Sintering with Reduction, *Phys. Mesomech*., 2023, vol. 26, pp. 39–47.

[2] M. Anisimova, A. Knyazeva, Basic models of phase formation at the mesolevel under reactive sintering of Ti-Al-Fe_2O_3 powder mixture, in: D. Sorokin, A. Grishkov (Eds.), *Proceeding of 8th International Congress on Energy Fluxes and Radiation Effects (EFRE 2022)*, Institute of High Current Electronics SB RAS, HCEI SB RAS, 2022.

[3] E.L. Shvedkov, E.T. Denisenko, Kovensky I.I., *Slovar-spravochnik po poroshkovoy metallurgii* [Dictionary-handbook of powder metallurgy], Naukova dumka Publ., Kyiv, 1982 (in Russian).

[4] M. Kizilyalli, J. Corish, R. Metselaar, Definitions of terms for diffusion in the solid state, *Pure Appl. Chem.*, 1999, vol. 71, no. 7, pp. 1307–1325.

[5] V.N. Chebotin, *Chemical diffusion in solids*, Nauka, Moscow, 1989 (in Russian).

[6] V.I. Dybkov, *Solid state reaction kinetics*, IPMS Publications, Kyev, 2013.

[7] A.M. Gusak, T.V. Zaporozhets, Y.O. Lyashenko, S.V. Kornienko, M.O. Pasichnyy, A.S. Shirinyan, *Diffusion-Controlled Solid State Reactions: In Alloys, Thin-Films, and Nanosystems*, John Wiley and Sons, New York, 2010.

[8] J. Svoboda, F.D Fischer, A new computational treatment of reactive diffusion in binary systems, *Comput. Mater. Sci.*, 2013, vol. 78, pp. 39–46.

[9] Y.M. Grigor'ev, S.L. Kharatyan, Z.S.Andrianova, A.N. Ivanova, A.G. Merzhanov, Diffusion kinetics of interaction of metals with gases, *Combust. Explos. Shock Waves*, 1977, vol. 13, pp. 604–610.

[10] Y.M. Grigor'ev, S.L. Kharatyan, Z.S. Andrianova, A.N. Ivanova, A.G. Merzhanov, Theory of reaction diffusion for bodies of plane, cylindrical, and spherical symmetry, *J. Eng. Phys.*, 1977, vol. 33, pp. 1353–1358.

[11] J. Benar, *Oxidation of Metals*, Metallurgiya, Moscow, 1968 (in Russian).

[12] J. Svoboda, F.D. Fischer, P. Fratzl, Diffusion and creep in multi-component alloys with non-ideal sources and sinks for vacancies, *Acta Mater*., 2006, vol. 54, no. 11, pp. 3043–3053.

[13] K.P. Gurov, E.A. Smirnov, A.N. Shabalin, *Diffuziya i kinetika fazovykh prevrashcheniy v metallakh i splavakh* [Diffusion and kinetics of phase transformations in metals and alloys], MEPHI, Moscow, 1990 (in Russian).

[14] B.Ya. Lyubov, *Kinetic Theory of Phase Transformations*, Amerind Pub., New Delhi, 1978.

[15] G.D.C. Kuiken, *Thermodynamics of irreversible processes. Applicationa to diffusion and rheology*, J. Wiley and Sons, Chichester, 1994.

[16] I. Kaur, W. Gust. *Fundamentals of Grain and Interphase Boundary Diffusion*, Ziegler Press, Stuttgart, 1989.

[17] Y.L. Corcoran, A.H. King, N. de Lanerolle, B. Kim, Grain Boundary Diffusion Layers on Silicon and Growth of Titanium Silicide, *J. Electron. Mater.*, 1990, vol.19, pp. 1177–1183.

[18] H.H. Farrell, G.H. Glimer, M. Suenaga, Grain boundary diffusion and growth of intermetallic layers, *J. Appl. Phys.*, 1974, vol. 45, no. 9, pp. 4025–4035.

[19] A. Furuto, M. Kajihara, Numerical Analysis for Kinetics of Reactive Diffusion Controlled by Boundary and Volume Diffusion in a Hypothetical Binary System, *Mater. Trans.*, 2008, vol. 49, no. 2, pp. 294-303.

[20] D.L. Bekea, Yu. Kaganovskii, G.L. Katona, Interdiffusion along grain boundaries – Diffusion induced grain boundary migration, low temperature homogenization and reactions in nanostructured thin films, *Prog. Mater. Sci.*, 2018, vol. 98, pp. 625–674.

[21] A.M. Gusak, Flux-Driven Lateral Grain Growth during Reactive Diffusion, *Metallofiz. Noveishie Tekhnol.*, 2020, vol. 42, no. 10, pp. 1335–1346.

[22] M.V. Chepak-Gizbrekht, A.G. Knyazeva, Two-dimensional model of grain boundary diffusion and oxidation, *PNRPU Mechanics Bulletin*, 2022, no. 1, pp. 156–166.

[23] M.V. Chepak-Gizbrekht, A.G. Knyazeva, Oxidation of TiAl alloy by oxygen grain boundary diffusion, *Intermetallics*, 2023, vol. 162, art. no. 107993.

[24] M.V. Chepak-Gizbrekht, A.G. Knyazeva, Modeling the oxidation process of TiAl and Ti_3Al intermetallic compounds due to grain-boundary diffusion of oxygen, *Uchenye Zapiski Kazanskogo Universiteta. Seriya Fiziko-Matematicheskie Nauki*, 2023, vol. 165, no 3, pp. 307-321 (in Russian).

[25] A. Knyazeva, O. Kryukova, A. Maslov, Two-level model of the grain boundary diffusion under electron beam action, *Comput. Mater. Sci*., 2021, vol. 196, art. no. 110548.
[26] G. Wang, B. Gleeson, D.L. Douglass, Phenomenological Treatment of Multilayer Growth, *Oxid Met*., 1989, vol. 31, no. 5–6, pp. 415–429.
[27] B. Cockeram, G. Wang, The influence of multi-layered kinetics on the selection of the primary phase during the diffusion-controlled growth of titanium-silicide layers, *Thin Solid Films*, 1995, vol. 269, no. 1–2, pp. 57–63.
[28] G.-X. Li, C.W. Powell, Theory of reaction diffusion in binary systems, *Acta Metall*., 1985, vol. 33, no. 1, pp. 23–31.
[29] V.I. Dybkov, Reaction diffusion in binary solid-solid, solid-liquid and solid-gaz sestems: common and distinctive features, *Defect Diffus Forum*, 2001, vol. 194–199, pp. 1503–1533.
[30] U. Gösele; K.N. Tu, "Critical thickness" of amorphous phase formation in binary diffusion couples, *J. Appl. Phys.*, 1989, vol. 66, no. 6, pp. 2619–2626.
[31] M. Kajihara, Influence of Temperature Dependence of Solubility on Kinetics for Reactive Diffusion in a Hypothetical Binary System, *Mater. Trans.*, 2008, vol. 49, no. 4, pp. 715–722.
[32] M. Kajihara, Analysis of kinetics of reactive diffusion in a hypothetical binary system, *Acta Mater*., 2004, vol. 52, no. 5, pp. 1193–1200.
[33] M. Danielewski, B. Wierzba, A. Gusak, M. Pawełkiewicz, J. Janczak-Rusch, Chemical interdiffusion in binary systems; interface barriers and phase competition, *J. Appl. Phys.*, 2011, vol. 110, no. 12, art. no. 123705.
[34] J. Svoboda, F.D. Fischer, Incorporation of vacancy generation/annihilation into reactive diffusion concept – Prediction of possible Kirkendall porosity, *Comput. Mater. Sci.*, 2017, vol. 127, pp. 136–140.
[35] A.V. Nazarov, K.P. Gurov. Kinetic theory of mutual diffusion in a binary system. Concentration of vacancies during mutual diffusion, *The Physics of Metals and Metallography*, 1974, vol. 37, no. 3, pp. 41–47.
[36] Yu.E. Ugaste, Kinetics of phase growth during mutual diffusion in multiphase binary systems, *Physics and Chemistry of Materials Treatment*, 1979, no. 3, pp.125–131 (in Russian).
[37] A.G. Knyazeva, M.A. Anisimova, E.N. Korosteleva, Features of diffusion-controlled processes of regulated volumetric synthesis from powder mixtures Ti–Al–Fe–Fe_2O_3, *PNRPU Mechanics Bulletin*, 2022, no. 3, pp. 125–134.
[38] E.N. Korosteleva, A.G.Knyazeva, M.A. Anisimova, I.O. Nikolaev, The impact of impurities on the Al–Fe–C system phase composition changes during sintering, *Powder Metallurgy and Functional Coatings*, 2023, vol. 17, no. 2, pp. 5–13.
[39] M.A. Anisimova, A.G.Knyazeva, E.N. Korosteleva, I.O. Nikolaev, Phase formation during composite synthesis under conditions of reactive sintering of the Ti+Al+Fe_2O_3+(Fe+C) powder mixture, *Izvestiya Vuzov. Fizika*, 2023, vol. 66, no 11, pp. 7–16 (in Russian).
[40] Y. Zhao, Y. Chen, S. Ai, D. Fang, A diffusion, oxidation reaction and large viscoelastic deformation coupled model with applications to SiC fiber oxidation, *Int. J. Plast.*, 2019, vol. 118, pp. 173–189.
[41] B.E. Deal, A.S. Grove, General relationship for the thermal oxidation of silicon, *J. Appl. Phys.*, 1965, vol.36, no. 12, pp. 3770–3778.
[42] M. Wilson, E. Opila, A review of SiC fiber oxidation with a new study of Hi-Nicalon SiC fiber oxidation, *Adv. Eng. Mater*., 2016, vol. 18, no. 10, pp. 1698–1709.
[43] W.L. Wang, S. Lee; J.R. Chen, Effect of chemical stress on diffusion in a hollow cylinder, *J. Appl. Phys*., 2002, vol. 91, no. 12, pp. 9584–9590.
[44] H. Haftbaradaran, J. Song, W.A. Curtin, H. Gao, Continuum and atomistic models of strongly coupled diffusion, stress, and solute concentration, *J. Power Sources*, 2011, vol. 196, no. 1, pp. 361–370.
[45] Z. Erdélyi, G. Schmitz, Reactive diffusion and stresses in spherical geometry, *Acta Mater*., 2012, vol. 60, no. 4, pp. 1807–1817.
[46] M. Roussel, Z. Erdélyi, G. Schmitz, Reactive diffusion and stresses in nanowires or nanorods, *Acta Mater.*, 2017, vol. 131, pp. 315–322.
[47] B.L. Hess, J.J. Ague, Diffusion-induced stress in crystals: Implications for timescales of mountain building, *Lithos*, 2024, vol. 488–489, art. no. 107783.

[48] B.L. Hess, J.J. Ague, Modeling diffusion in ionic, crystalline solids with internal stress gradients, *Geochim. Cosmochim. Acta*, 2023, vol. 354, pp. 27–37.
[49] H. Yang, F. Fan, W. Liang, X. Guo, T. Zhu, S. Zhang, A chemo-mechanical model of lithiation in silicon, *J. Mech. Phys. Solids*, 2014, vol. 70, pp. 349–361.
[50] D. Clerici, F. Mocera, A. Somà, Analytical Solution for Coupled Diffusion Induced Stress Model for Lithium-Ion Battery, *Energies*, 2020, vol. 13, no.7, art. no. 1717.
[51] I.V. Belova, G.E. Murch, Thermal and diffusion-induced stresses in crystalline solids, *J. Appl. Phys.*, 1995, vol. 77, no. 1, pp. 127–134.
[52] R. Deshpande, Y.-T. Cheng, M.W. Verbrugge, Modeling diffusion-induced stress in nanowire electrode structures, *J. Power Sources*, 2010, vol. 195, no. 15, pp. 5081–5088.
[53] Z. Guo, T. Zhang, H. Hu, Y. Song, J. Zhang, Effects of Hydrostatic Stress and Concentration-Dependent Elastic Modulus on Diffusion-Induced Stresses in Cylindrical Li-Ion Batteries, *J. Appl. Mech.*, 2014, vol. 81, no. 3, art. no. 031013.
[54] J.L. Chu, S. Lee, The effect of chemical stresses on diffusion, *J. Appl. Phys.*, 1994, vol. 75, no. 6, pp. 2823–2829.
[55] Ya.S. Podstrigach, Diffusion theory of the anelasticity of metals, *J. Appl. Mech. Tech. Phys.*, 1965, vol. 6, pp. 56–60.
[56] F.C. Larche, J.W. Cahn, The effect of self-stress on diffusion in solids, *Acta Metall*., 1982, vol. 30, no. 10, pp. 1835–1845.
[57] F.C. Larche, J.W. Cahn, The Interactions of Composition and Stress in Crystalline Solids, *Journal of Research of the National Bureau of Standards*, 1984, vol. 89, no.6, pp. 467–500.
[58] F.C. Larche, J.W. Cahn, Thermochemical equilibrium of multiphase solid under stress, *Acta Metall*., 1987, vol. 26, no. 10, pp. 1579–1589.
[59] E.C. Aifantis, On the problem of diffusion in solids, *Acta Mech*., 1980, vol. 37, pp. 265–296.
[60] V.S. Eremeev, *Diffusion and Stresses*, Energoatomizdat, Moscow, 1984 (in Russian).
[61] J.-L. Grosseau-Poussard, B. Panicaud, S. Ben Afia, Modelling of stresses evolution in growing thermal oxides on metals. A methodology to identify the corresponding mechanical parameters, *Comput. Mater. Sci.*, 2013, vol. 71, pp. 47–55.
[62] Sh. Geng, K. Zhang, B. Zheng, Yu. Zhang, Effects of concentration-dependent modulus and external loads on Li-ion diffusion and stress distribution in a bilayer electrode, *Acta Mech*., 2024, vol. 235, pp. 191–201.
[63] Z. Cui, F. Gao, J. Qu, A finite deformation stress-dependent chemical potential and its applications to lithium ion batteries, *J. Mech. Phys. Solid.*, 2012, vol. 60, no. 7, pp. 1280–1295.
[64] J.L. Bouvard, D.K. Francis, M.A. Tschopp, E.B. Marin, D.J. Bammann, M.F. Horstemeyer, An internal state variable material model for predicting the time, thermomechanical, and stress state dependence of amorphous glassy polymers under large deformation, *Int. J. Plast*., 2013, vol. 42, pp. 168–193.
[65] X. Zhang, Q.J. Wang, H. Shen, A multi-field coupled mechanical-electric-magnetic-chemical-thermal (MEMCT) theory for material systems. *Comput. Method Appl. Mech. Eng.*, 2018, vol. 341, pp. 133–162.
[66] X. Zhang, Z. Zhong, A coupled theory for chemically active and deformable solids with mass diffusion and heat conduction, *J. Mech. Phys. Solids*, 2017, vol. 107, pp. 49–75.
[67] I. Gyarmati, *Non-equilibrium Thermodynamics. Field Theory and Variational Principles*, Springer-Verlag, Berlin, 1970.
[68] S.R. De Groot, P. Mazur, *Non-Equilibrium Thermodynamics*, Dover, New York, 1984
[69] R. Haase, *Thermodynamics of Irreversible Processes*, Dover, New York, 1969
[70] W. Liu, S. Shen, Coupled chemomechanical theory with strain gradient and surface effects. *Acta Mech*., 2018, vol. 229, pp. 133–147.
[71] G. Rambert, J. Grandidier, E. Aifantis, On the direct interactions between heat transfer, mass transport and chemical processes within gradient elasticity, *Eur. J. Mech. A*, 2007, vol. 26, no. 1, pp. 68–87.
[72] K.P. Frolova, E.N. Vilchevskaya, V.A. Polyanskiy, Yu.A. Yakovlev, Modeling the skin effect associated with hydrogen accumulation by means of the micropolar continuum, *Contin. Mech. Thermodyn*., 2021, vol. 33, pp. 697–711.

[73] P. Grigoreva, E.N. Vilchevskaya, W.H. Müller, Stress and Diffusion Assisted Chemical Reaction Front Kinetics in Cylindrical Structures, in: H. Altenbach, H. Irschik, V. Matveenko (Eds.), *Contributions to Advanced Dynamics and Continuum Mechanics. Advanced Structured Materials*, *vol 114*, Springer, Cham, 2019, pp 53–72.
[74] A.B. Freidin, I.K. Korolev, S.P. Aleshchenko, E.N. Vilchevskaya, Chemical affinity tensor and chemical reaction front propagation: theory and FE-simulations. *Int. J. Fract*., 2016, vol. 202, pp. 245–259.
[75] A.B. Freidin, I.K. Korolev, E.N. Vilchevskaya, Stress-assist chemical reactions front propagation in deformable solids, *Int. J. Eng. Sci*., 2014, vol. 83, pp. 57–75.
[76] A. Gusak, N. Storozhuk, Diffusion-Controlled Phase Transformations in Open Systems, in: A. Paul, S. Divinski (Eds.), *Handbook of Solid State Diffusion, vol. 2*, Elsevier, Amsterdam, 2017, pp. 37–100.
[77] R.-H. Fan, H.-L. Lu, K.-N. Sun, W.-X. Wang, X.-B Yi, Kinetics of thermite reaction in Al-Fe_2O_3 system, *Thermochim. Acta*, 2006, vol. 440, no. 2, pp. 129–131.
[78] H.A. Wriedt, The Al-O (Aluminum-Oxygen) system, *Bulletin of Alloy Phase Diagrams*, 1985, vol. 6, pp. 548–553.
[79] J.L. Murray, Fe–Al binary phase diagram, in: H. Baker (Ed.), *Alloy Phase Diagrams*, *vol. 3*, ASM International, Ohio, 1992, p. 54.
[80] O.K. Goldbeck, *Iron—binary phase diagrams*, Springer, Berlin, 1982
[81] S.V. Shukhardin, *Binary and Multicomponent Systems Based on Copper*, Nauka, Moscow, 1979 (in Russian).
[82] N.P. Lyakishev, Phase Diagrams of Binary Metal System, Metallurgiya, Moscow, 1997.
[83] Y. Nakamura, K. Sumiyama, H. Ezawa, Vapor quenched Fe-Ti alloys: Formation of amorphous phase, and metastable Ti_2Fe phase by aging, *Hyperfine Interact*., 1986, vol. 27, pp. 361–364.
[84] S.K. Misra, M. Kahrizi, K. Singh, N. Venkatramani, D. Bahadur, EPR, X-ray, and magnetization studies of metastable alloys Ti_2Fe, $Al_{40}Cu_{10}Mn_{25}Ge_{25}$ and $Al_{65}Cu_{20}Fe_{15}$ as prepared by mechanical alloying, *J. Magn. Magn. Mater*., 1995, vol. 150, no. 3, pp. 430-436.
[85] Y.-Ch. Lin, A.S. Shteinberg, P.J. McGinn, A.S. Mukasyan, Kinetics study in Ti-Fe_2O_3 system by electro-thermal explosion method, *Int. J. Therm. Sci*., 2014, vol. 84, pp. 369–378.
[86] B.A. Boley, J.H. Weiner, *Theory of Thermal Stresses*, Wiley, New York, 1960
[87] M. Anisimova, A. Knyazeva, Diffusion Interaction Model in Al-Fe_2O_3 System with Including the Formation of Intermetallic Phases, *Interfacial Phenom. Heat Transf.*, 2024, vol. 12, no. 1, pp. 75–88.
[88] V.N. Antsiferov, V.G. Gilev, The role of bulk and mass effects of reactions in reaction sintering processes, *Powder Metallurgy and Functional Coatings,* 2015, no. 4, pp. 9–20.
[89] L.N. Larikov, Mechanisms of reactive mutual diffusion (review), *Metallofiz. Noveishie Tekhnologii*, 1994, vol. 16, no. 9, pp. 3–27.
[90] V.I. Arkharov, On the kinetics of reaction diffusion in systems with several intermediate phases, *Physics of Metals and Metallography*, 1959, vol. 8, no. 2, pp. 193–204.