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**A unified thermodynamic framework for the modelling of diffusive and displacive phase transitions.** (English) Zbl 1423.80023

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Summary: A thermodynamically consistent framework able to model both diffusive and displacive phase transitions is proposed. The first law of thermodynamics, the balance of linear momentum equation (in the linearized strain approximation) and the Cahn-Hilliard equation for solute mass conservation are the governing equations of the model, which is complemented by a suitable choice of the Helmholtz free energy and consistent boundary and initial conditions. To highlight thermo-chemo-mechanical interactions, some numerical tests are performed in which the phase transition is triggered by setting the value of the initial temperature; a time-temperature-transformation diagram is determined.

**MSC:**

80A22 Stefan problems, phase changes, etc.



**Keywords:**

diffusive phase transition; displacive phase transition; thermodynamics; phase field model

**Software:**

DOLFIN

**Full Text:** DOI

**References:**

[1] Ahluwalia, R.; Lookman, T.; Saxena, A., Dynamic strain loading of cubic to tetragonal martensites, Acta materialia, 54, 2109-2120, (2006)

[2] Albers, R.C.; Ahluwalia, R.; Lookman, T.; Saxena, A., Modeling solid – solid phase transformations: from single crystal to polycrystal behaviour, Computational and applied mathematics, 23, 345-361, (2004) · Zbl 1213.74055

[3] Alt, H.W.; Pawlow, I., A mathematical model of dynamics of non-isothermal phase separation, Physica D, 59, 389-416, (1992) · Zbl 0763.58031

[4] Artemev, A.; Jin, Y.; Khachaturyan, A., Three-dimensional phase field model of proper martensitic transformation, Acta materialia, 49, 7, 1165-1177, (2001)

[5] Barsch, G.R.; Krumhansl, J.A., Twin boundaries in ferroelastic media without interface dislocations, Physical review letters, 53, 1070-1072, (1984)

[6] Berti, V.; Fabrizio, M.; Grandi, D., Phase transitions in shape memory alloys: A non-isothermal ginzburg – landau model, Physica D, 239, 1-2, 95-102, (2010) · Zbl 1189.82081

[7] Bhadeshia, H. K. D. H. (1987). \textit{Worked examples in the geometry of crystals}. The Institute of Metals. London.

[8] Bouville, M.; Ahluwalia, R., Effect of lattice-mismatch-induced strains on coupled diffusive and displacive phase transformations, Physical review B, 75, 054110-1-054110-11, (2007)

[9] Brokate, M.; Sprekels, J., Hysteresis and phase transitions, (1996), Springer New York · Zbl 0951.74002

[10] Cahn, J., On spinodal decomposition, Acta metallurgica, 9, 795-801, (1961)

[11] Cahn, J.; Hilliard, J.E., Free energy of a nonuniform system. I: interfacial free energy, Journal of chemical physics, 28, 2, 258-267, (1958)

[12] Falk, F., Model free energy, mechanics and thermodynamics of shape memory alloys, Acta metallurgica, 28, 1773-1780, (1980)

[13] Fried, E.; Gurtin, M.E., Continuum theory of thermally induced phase transitions based on an order parameter, Physica D, 68, R 326-R 343, (1993) · Zbl 0793.35049

[14] Gurtin, M.E., Generalized ginzburg – landau and cahn – hilliard equations by a microforce balance, Physica D, 92, 178-192, (1996) · Zbl 0885.35121

[15] Hoemberg, D., A mathematical model for the phase transitions in eutectoid carbon steel, IMA journal of applied mathematics, 54, 31-57, (1995) · Zbl 0830.65126

[16] Landau, L.D.; Lifshitz, D.M., Statistical physics, (1968), Pergamon Oxford

[17] Levitas, V.I., Thermomechanical and kinetic approaches to diffusional – displacive phase transitions in inelastic materials, Mechanics research communications, 27, 217-227, (2000) · Zbl 0965.74047

[18] Levitas, V.I.; Preston, D.L., Three-dimensional Landau theory for multivariant stress-induced martensitic phase transformations. I: austenite⊠martensite, Physical review B, 66, 134206-1-134206-9, (2002)

[19] Lieberman, D.S.; Wechsler, M.S.; Read, T.A., Cubic to orthorhombic diffusionless phase change-experimental and theoretical studies of aucd, Journal of applied physics, 26, 473-484, (1955)

[20] Logg, A.; Wells, G.N., DOLFIN: automated finite element computing, ACM transactions on mathematical software, 37, 2, (2010), Article 20, 28 pages · Zbl 1364.65254

[21] (), Vol. 7

[22] Maraldi, M.; Wells, G.N.; Molari, L., Phase field model for coupled displacive and diffusive microstructural processes under thermal loading, \textit{journal of the mechanics and physics of solids}, 59, 8, 1596-1612, (2011) · Zbl 1270.74159

[23] Onuki, A.; Furukawa, A., Phase transitions of binary alloys with elastic inhomogeneity, Physical review letter, 83, 452-455, (2001)

[24] Polizzotto, C., Unified thermodynamic framework for nonlocal/gradient continuum theories, European journal mechanics A/solids, 22, 651-668, (2003) · Zbl 1032.74505

[25] Rao, M.; Sengupta, S., Nucleation of solids in solids: ferrites and martensites, Physical review letter, 91, 045502-1-045502-3, (2003)

[26] Shenoy, S.R.; Lookman, T.; Saxena, A.; Bishop, A.R., Martensitic textures: multiscale consequences of elastic compatibility, Physical review B, 60, (1999), R 12-537-541

[27] Toledano, J.C.; Toledano, P., The Landau theory of the phase transitions, (1987), World Scientific Editor

[28] Wang, Y.Z.; Chen, L.Q.; Khachaturyan, A.G., Shape evolution of a coherent tetragonal precipitate in partially-stabilized cubic zro2-a computer-simulation, Journal of American ceramic society, 76, 12, 3029-3033, (1993)

[29] Wang, Y.; Khachaturyan, A.G., Three dimensional field model and computer modeling of martensitic transformations, Acta materialia, 45, 759-773, (1997)