Abstract for MSH Sept 2012

Using gradient structures for modeling semiconductors

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We show that classical energy-drift-diffusion systems used for modeling of semiconductor devices can be written as gradient systems in the form

$$\partial_t \mathbf{u} = -\mathcal{K}(\mathbf{u})\mathrm{D}\Phi(\mathbf{u}),$$

where $\mathbf{u}$ is a vector of densities of the different species and possibly the temperature (or the internal energy), cf. [Mie11]. While the potential Φ is the free energy in the isothermal case and the negative entropy in the temperature-dependent case, the Onsager operator $\mathcal{K}(\mathbf{u}) = G(\mathbf{u})^{-1}$ is the inverse of the metric tensor $\mathcal{G}$ and has an additive split into the different dissipation mechanics:

$$\mathcal{K}(\mathbf{u})\boldsymbol{\xi} = \mathcal{K}_{\mathrm{diff}}(\mathbf{u})\boldsymbol{\xi} + \mathcal{K}_{\mathrm{react}}(\mathbf{u})\boldsymbol{\xi} = -\mathrm{div}\big(\mathbb{M}(\mathbf{u})\nabla\boldsymbol{\xi}\big) + \mathbb{K}(\mathbf{u})\boldsymbol{\xi}.$$

In the case of Fermi-Dirac statistics this modeling lead to new and more consistent modeling of diffusion enhancement and reaction kinetics. In particular, the modeling of semiconductors via gradient system $(\Phi, \mathcal{K})$ yields always thermodynamically consistent models and highlights the different physical aspects of the theory in a clear way.

It is shown in [GlM12, Mie12] that gradient structures can also used effectively to model hybrid models with nontrivial bulk-interface interaction and active interfaces, which are need in photovoltaics. Finally, we discuss how the theory of geodesically λ-convex gradient can be applied in this field, cf. [LiM12].

[GlM12] A. Glitzky and A. Mielke. A gradient structure for systems coupling reaction-diffusion effects in bulk and interfaces. *Z. angew. Math. Phys. (ZAMP)*, 2012. To appear. WIAS preprint 1603 (April 2011, doi 10.1007/s00033-0012-207-y).

[LiM12] M. Liero and A. Mielke. Gradient structures and geodesic convexity for reaction-diffusion systems. Submitted. WIAS preprint 1701 (April 2012).

[Mie11] A. Mielke. A gradient structure for reaction-diffusion systems and for energy-drift-diffusion systems. *Nonlinearity*, 24, 1329–1346, 2011.

[Mie12] A. Mielke. Thermomechanical modeling of energy-reaction-diffusion systems, including bulk-interface interactions. *Discr. Cont. Dynam. Systems Ser. S*, 2012. To appear. WIAS preprint 1661 (Nov. 2011).