Strain Engineering for Functional Heterostructures: Aspects of Elasticity

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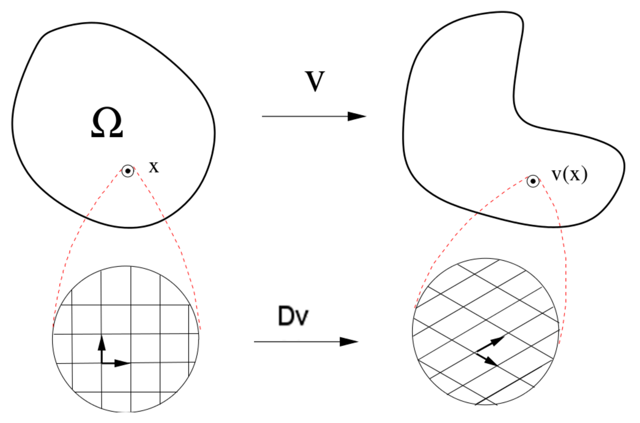
Summary

- Strain engineering for semiconductor devices or lithium-ion batteries requires a good understanding of elastic effects that strongly influence their functional properties
- Problems in the modeling of material systems related to:
  - Choice of free energy density with suitable properties
  - Dimension reduction for lower-dimensional structures
- In lower-dimensional structures, mathematical challenges arise due to the coupling of mechanical deformation with other physical effects such as electrostatics
- Use variational techniques, e.g., Γ-convergence, combined with modern tools for nonlinear partial differential equations

Polyconvex energy densities with generic elastic constants

Variational models of elasticity

- reference domain $\Omega \subseteq \mathbb{R}^n$
- deformation $v : \Omega \to \mathbb{R}^n$
- elastic energy $\int_\Omega W(\nabla v)\,dx \Rightarrow \min!$



Modeling assumptions for free energy density $W : \mathbb{R}^{n\times n} \to [0,\infty]$:

- *frame invariance:* $W(RF) = W(F)$ for all $R \in SO(n)$ and all $F \in \mathbb{R}^{n\times n}$
- *material symmetry:* For the point group $\mathcal{P} \subseteq O(n)$
  $W(P^T F P) = W(F)$ for all $P \in \mathcal{P}$ and all $F \in \mathbb{R}^{n\times n}$
- *normalization:* $W(F) \geq 0$ and $[W(F) = 0 \iff F \in SO(n)]$
- *existence* of minimizers: W polyconvex [Ball '77], i.e., there exists a convex and lower semi-continuous function $G : \mathbb{R}^{\tau(n)} \to [0,\infty]$ s.t.
  $$W(F) = G(T(F)), \qquad \text{where} \quad T(F) = (F, \det(F), \operatorname{cof}(F), \dots)$$
- *linearization and measured elastic constants:*
  $$W(\mathrm{Id} + \varepsilon) = W(\mathrm{Id}) + DW(\mathrm{Id})\varepsilon + \frac{1}{2}D^2W(\mathrm{Id})[\varepsilon,\varepsilon] + o(|\varepsilon|^2)$$
  $$= \frac{1}{2}\sum_{ijkl} \mathbb{C}_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + o(|\varepsilon|^2)$$
- *smoothness and non-interpenetration:* $W \in C^\infty(\mathbb{R}^{n\times n})$ or $W \in C^\infty(\mathbb{R}^{n\times n} \cap \{\det > 0\})$ and $W(F) \to \infty$ as $\det F \to 0$

Typical approaches in the literature

- linear elastic energy density evaluated at nonlinear strains [?], which leads to non-polyconvex W
- specific ansatz using structural tensors → restrictions on elastic constants

Result [Conti, Lenz & Zwicknagl, in preparation]:
Let P be a subgroup of $O(n)$, $\mathbb{C} : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ linear, symmetric s.t.
$$\mathbb{C}\xi : \xi \geq \tilde{c}|\xi + \xi^T|^2, \quad \mathbb{C}(\xi - \xi^T) = 0 \text{ for all } \xi \in \mathbb{R}^{n\times n},$$
$$\mathbb{C}(R\xi R^T) : (R\xi R^T) = \mathbb{C}\xi : \xi \text{ for all } \xi \in \mathbb{R}^{n\times n}, R \in P.$$
Then,
(i) there is a polyconvex function $W \in C^\infty(\mathbb{R}^{n\times n}; [0,\infty))$ s.t.
$$W(\xi) \geq c\,\mathrm{dist}^2(\xi, SO(n)), \quad \min W = W(Id) = 0, \quad D^2W(Id) = \mathbb{C}$$
and
$$W(QR^T\xi R) = W(\xi) \text{ for all } Q \in SO(n), R \in P, \xi \in \mathbb{R}^{n\times n}.$$
(ii) there is a polyconvex function $W \in C^\infty(\mathbb{R}^{n\times n} \cap \{\det > 0\}; [0,\infty))$ s.t. $W(\xi) \to \infty$ as $\det \xi \to 0$ and (i) holds.

Idea of the proof: Use linear elastic energy density evaluated at nonlinear strain near $SO(n)$, and construct explicit polyconvex extension using curvature of $SO(n)$.

Rigorous dimension reduction via Γ-convergence

Thin structures with thickness $0 < h \ll 1$

$$\text{plates} \quad \Omega_h^{\text{plate}} = \omega \times \left(-\tfrac{h}{2}, +\tfrac{h}{2}\right), \qquad \omega \subset \mathbb{R}^{n-1}$$
$$\text{rods} \quad \Omega_h^{\text{rod}} = (0, L) \times hS, \qquad S \subset \mathbb{R}^{n-1}$$

Finite-strain electro-mechanical model for deformation v and electric potential φ

$$-\operatorname{div}\big((\det M(x)\partial_F W(\nabla v M(x)^{-1})M(x)^{-\top} - h^\alpha \operatorname{div}\mathfrak{H}(\nabla^2 v)\big) = 0,$$
$$-\operatorname{div}(A(x, \nabla v)\nabla\varphi) = q(x),$$

- hyperstress regul. $\mathfrak{H}$ leads to 2nd-grade nonsimple materials
- prestrain $M(x) \in \mathbb{R}^{n\times n}$ models lattice mismatch in heterostructures
- $A(x,F) = (\det F)F^{-1}a(x)F^{-\top}$, $F = \nabla v$, is the pulled-back dielectric coefficient, $a \in L^\infty(\Omega_h)$ such that $a(x) \geq a_0 > 0$ a.e. in Ω_h, fixed charge density $q \in L^\infty(\Omega_h)$

System has saddle-point structure with energy functional

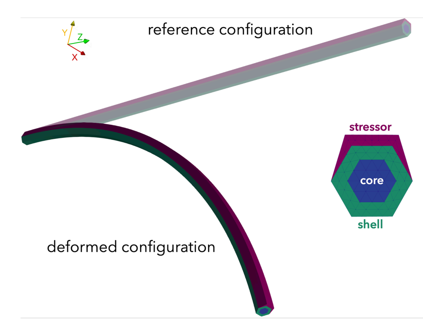
$$\mathcal{E}_h(v,\varphi) = \mathcal{E}_h^{\text{mech}}(v) - \mathcal{E}_h^{\text{elec}}(v,\varphi)$$
$$= \int_{\Omega_h} W(\nabla v M^{-1})\det M + h^\alpha H(\nabla^2 v) + q\varphi - \tfrac{1}{2}A(\nabla v)\nabla\varphi \cdot \nabla\varphi\,dx$$

Work in progress: Limit passage for $h \to 0$ for thin plate in the bending regime, i.e., for the scaling $\widetilde{\mathcal{E}}_h = \frac{1}{h^2}\mathcal{E}_h$ via Γ-convergence methods. At the first stage, we have proved the Γ− convergence result for bending model with prestrain coupled by the Poisson equation without deformation, $\nabla v = id$, and with isotropic permeability.

Outlook: Investigate rod model and different scaling regimes.

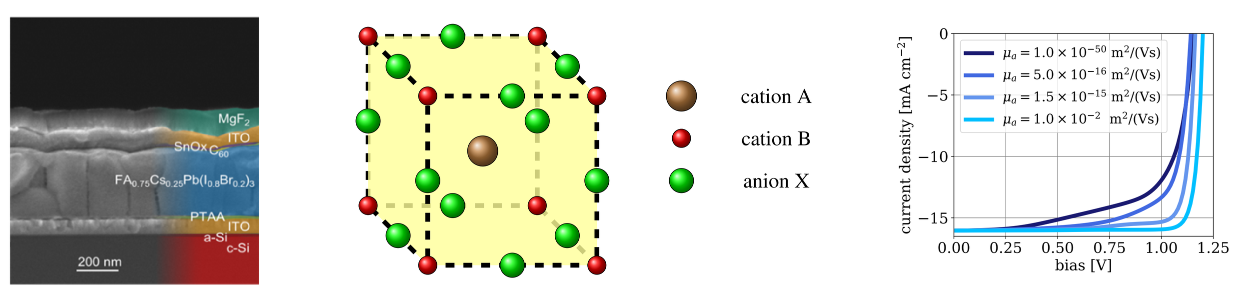
Strain distribution in zincblende and wurtzite GaAs nanowires

- mathematical model for heterostructures reacting on strain caused by lattice mismatch [?]
- non-linear elasticity with local prestrain
- simulations using finite element methods
- significant potential of strain to influence piezoelectricity and electronic band structure



Vacancy assisted charge transport (with PaA-1)

- Application: semiconductor/perovskite/semiconductor heterostructures for perovskite solar cells
- analysis of drift-diffusion models including the migration of ions: existence of weak solutions, boundedness [?], and uniqueness



Perovskite Silicon Tandem Solar Cell (Fraunhofer ISE, Freiburg), Perovskite unit cell, Current-Voltage-Characteristics

Cooperations

- S. Conti (Bonn), J. Ginster (WIAS), L. Abel (HUB), M. Rumpf (Bonn), M. Lenz (Bonn), Y. Hadjimichael (WIAS)
- AMaSiS 2024 workshop together with PaA-1, AA2-13, AA2-17
- Finite-strain hyperelasticity in battery models with PaA-2

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