

Multiphase transformation and mechanical analysis of Sn-based nanoparticle during lithiation process

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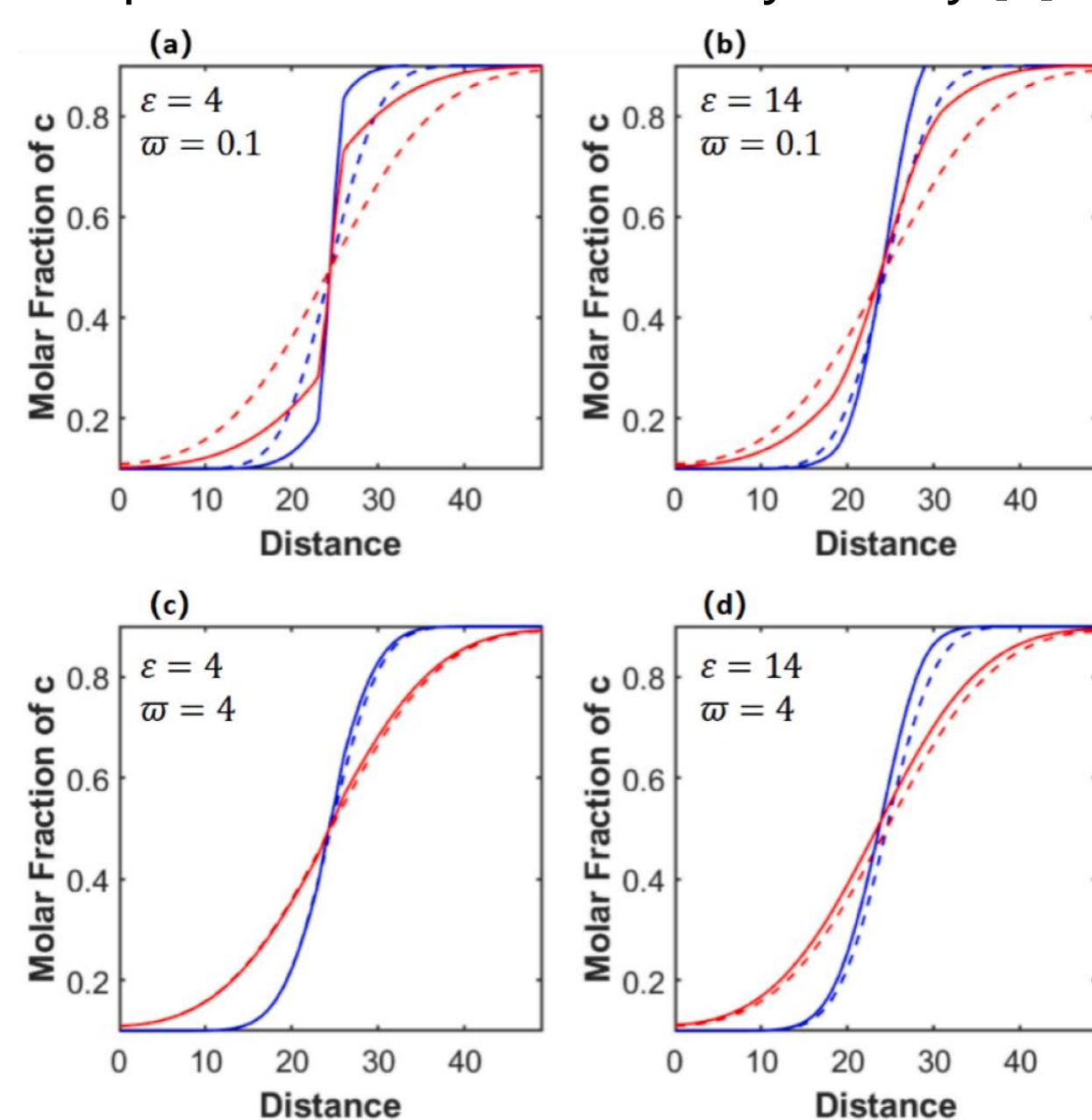
lithiation/delithiation process of Li_xSn ideal spherical nanoparticle

Methods

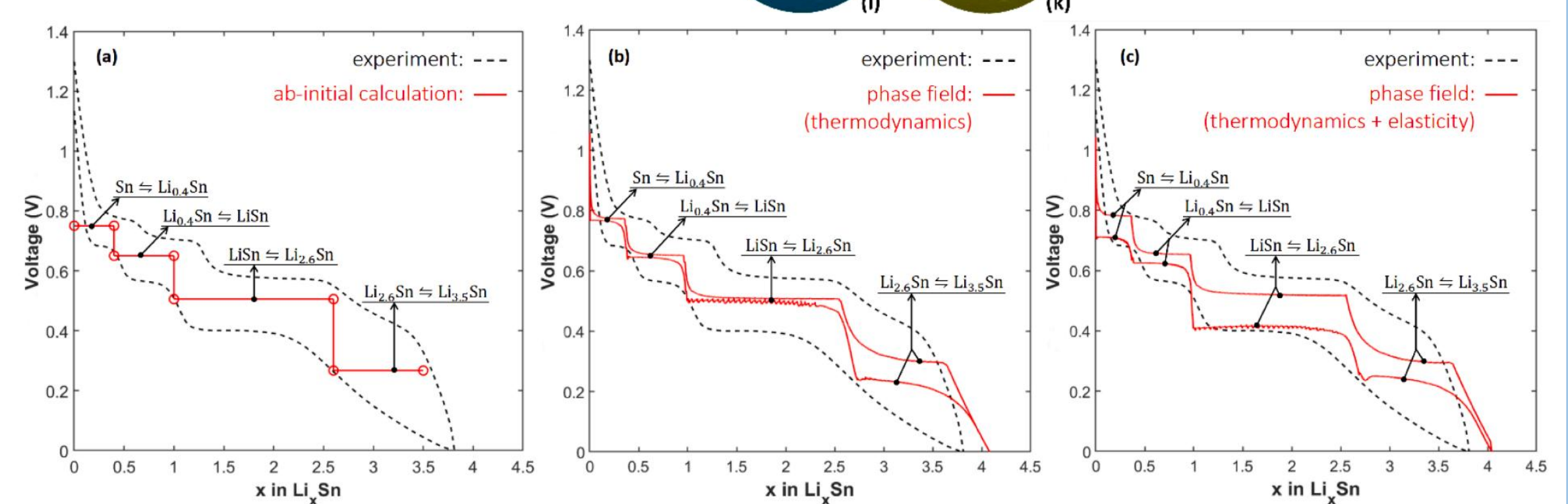
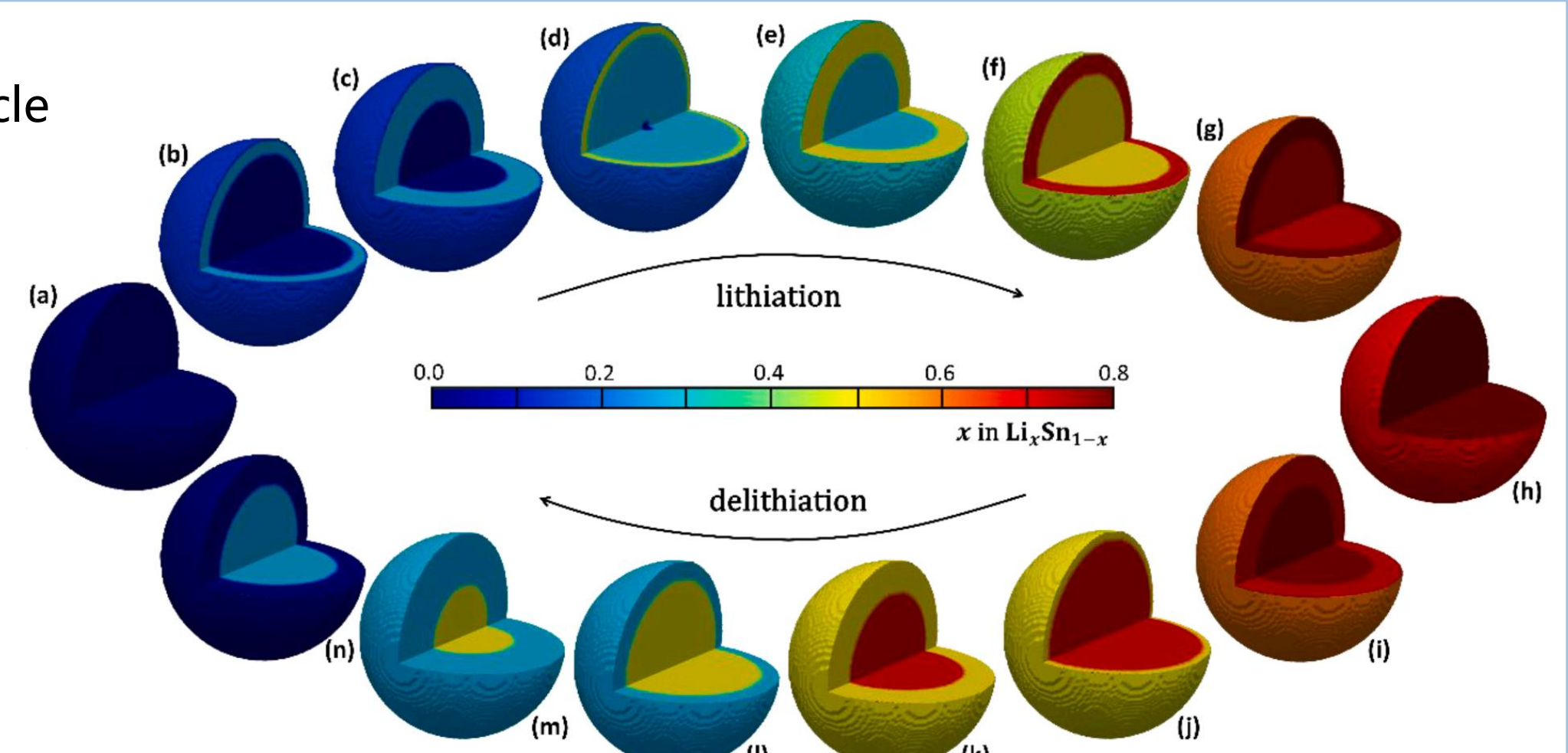
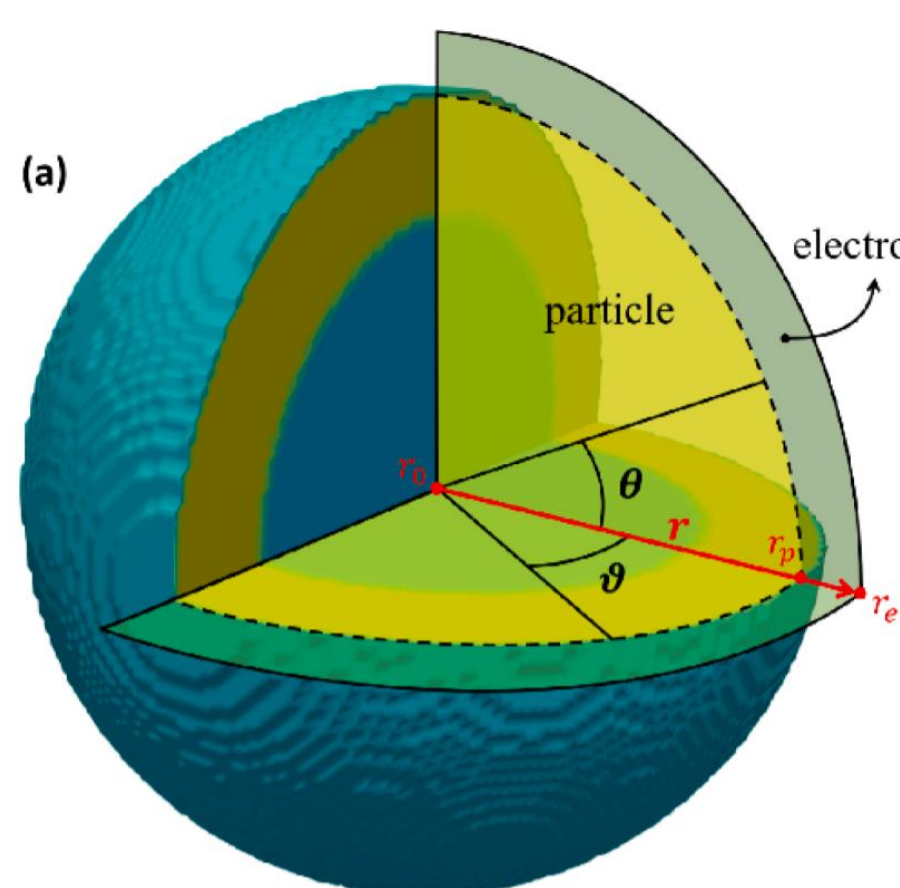
- multiphase-field method [1]
- multiphase concentration functional [2]
- phase-field microelasticity theory [3]

Applications

- modeling ideal spherical nanoparticle
- lithiation/delithiation cycling
- output voltage profile



compare multiphase concentration functional with mass-conservation equation



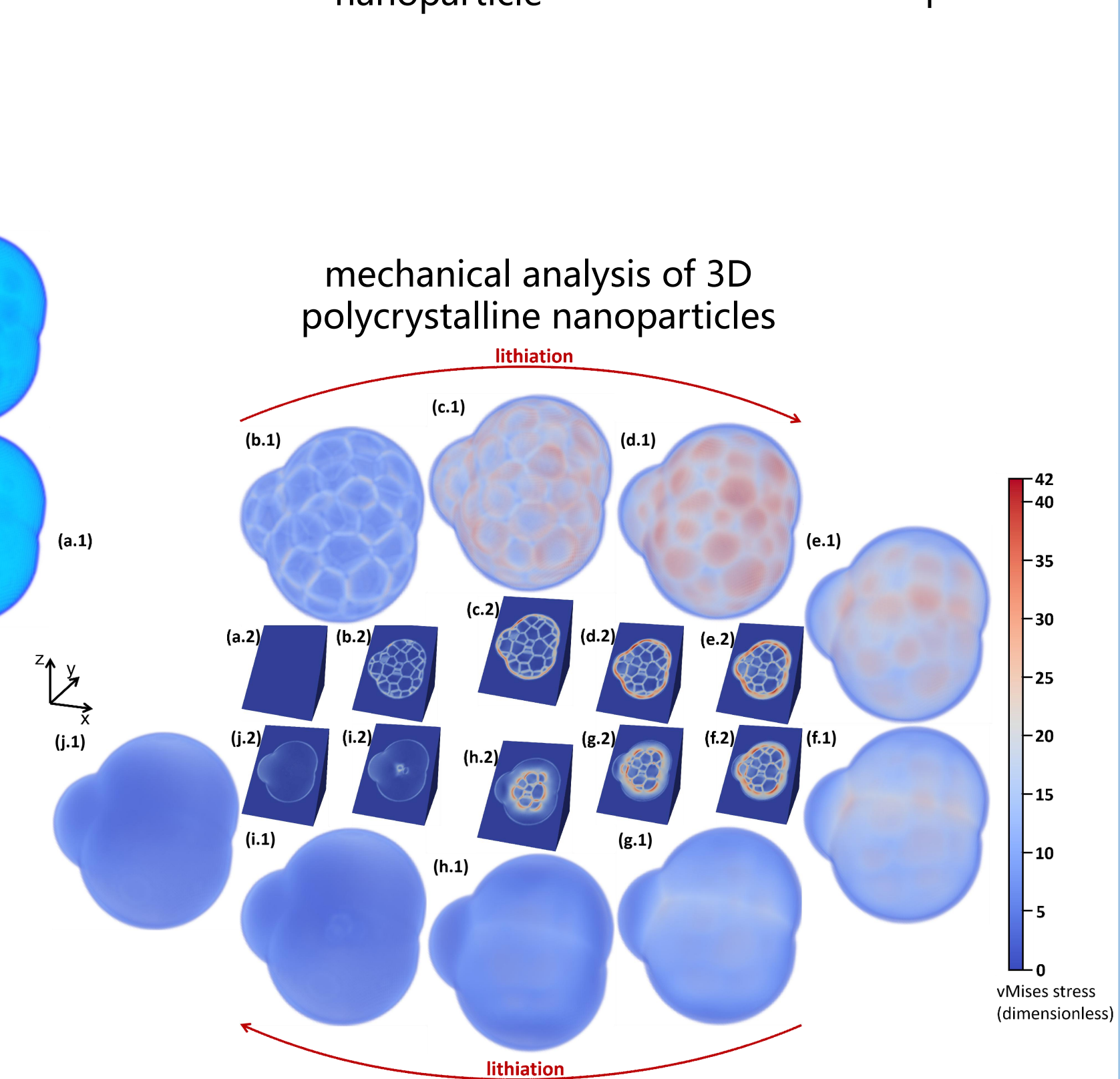
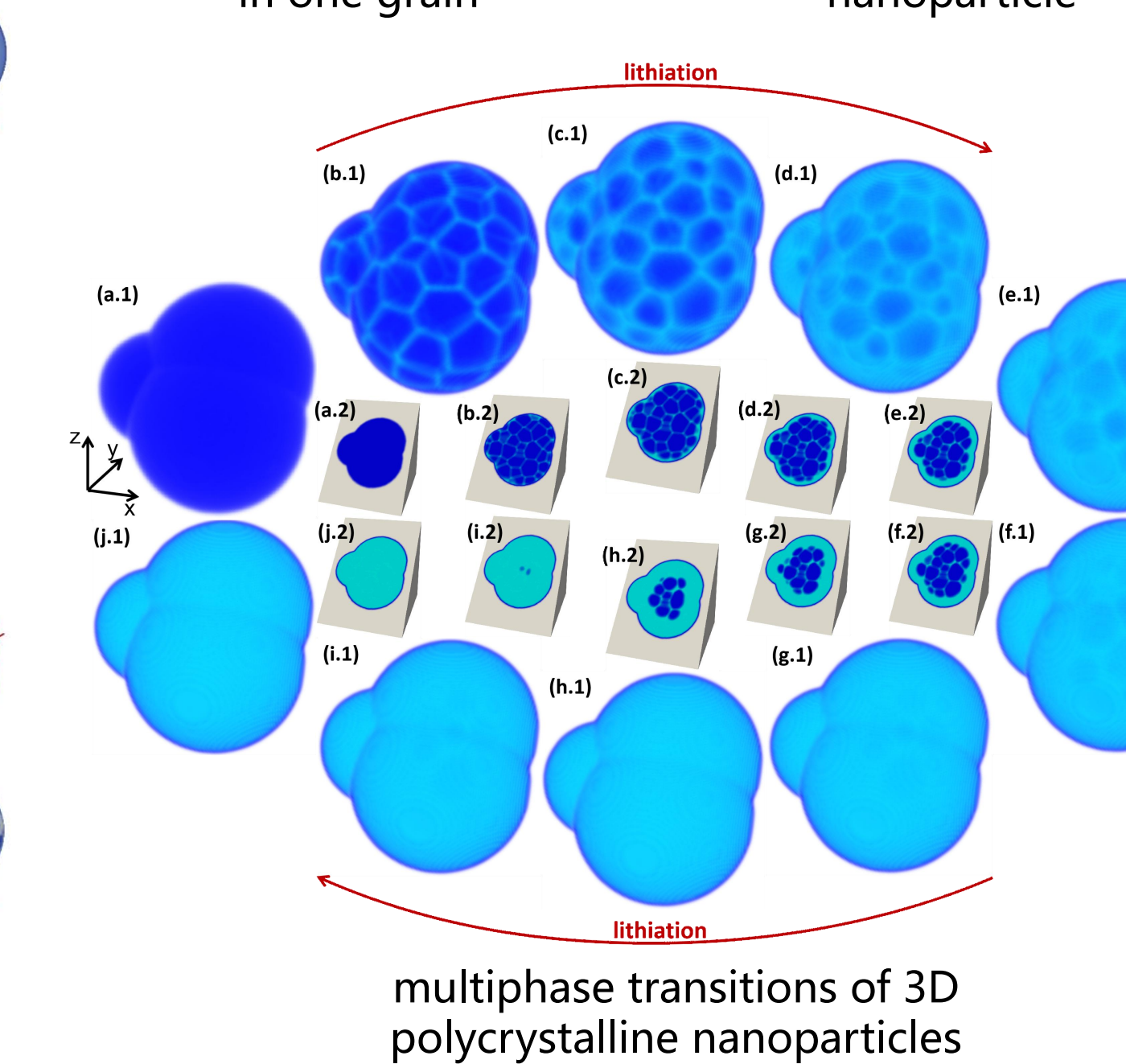
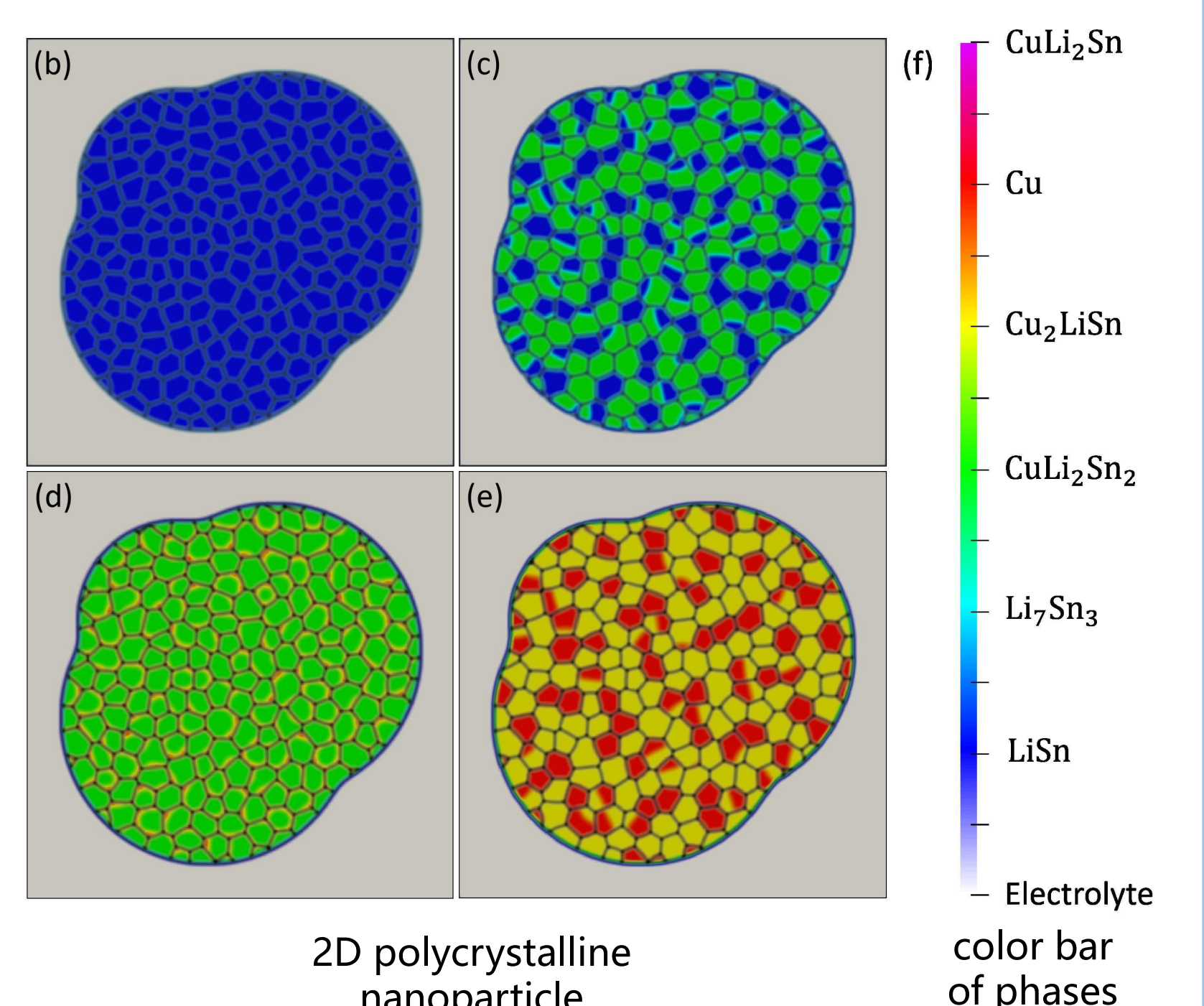
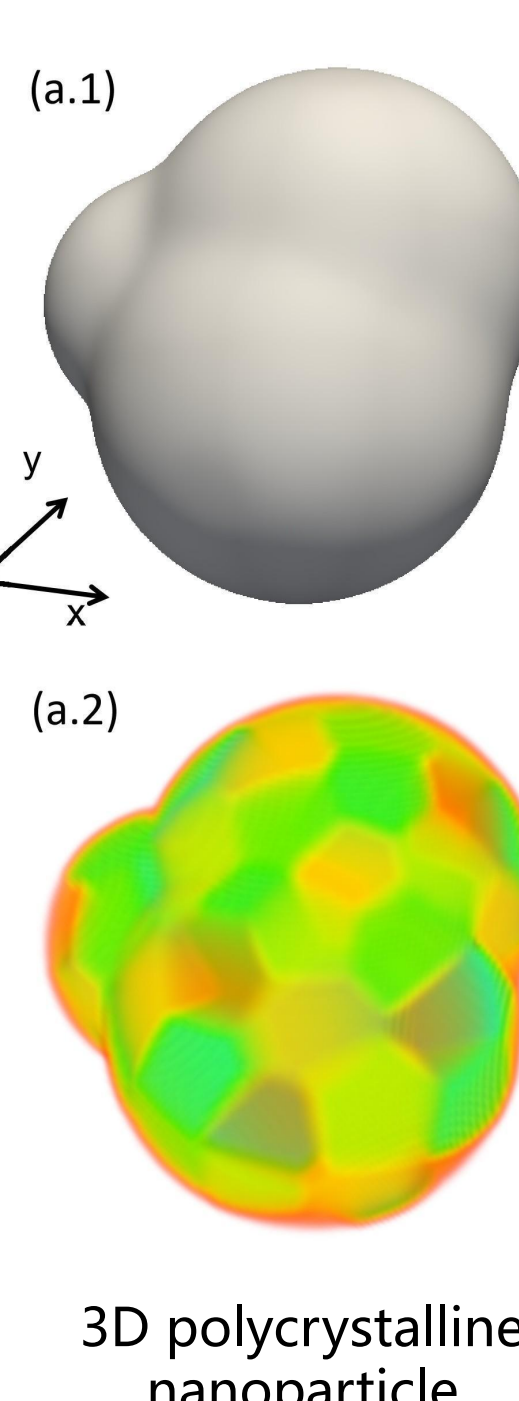
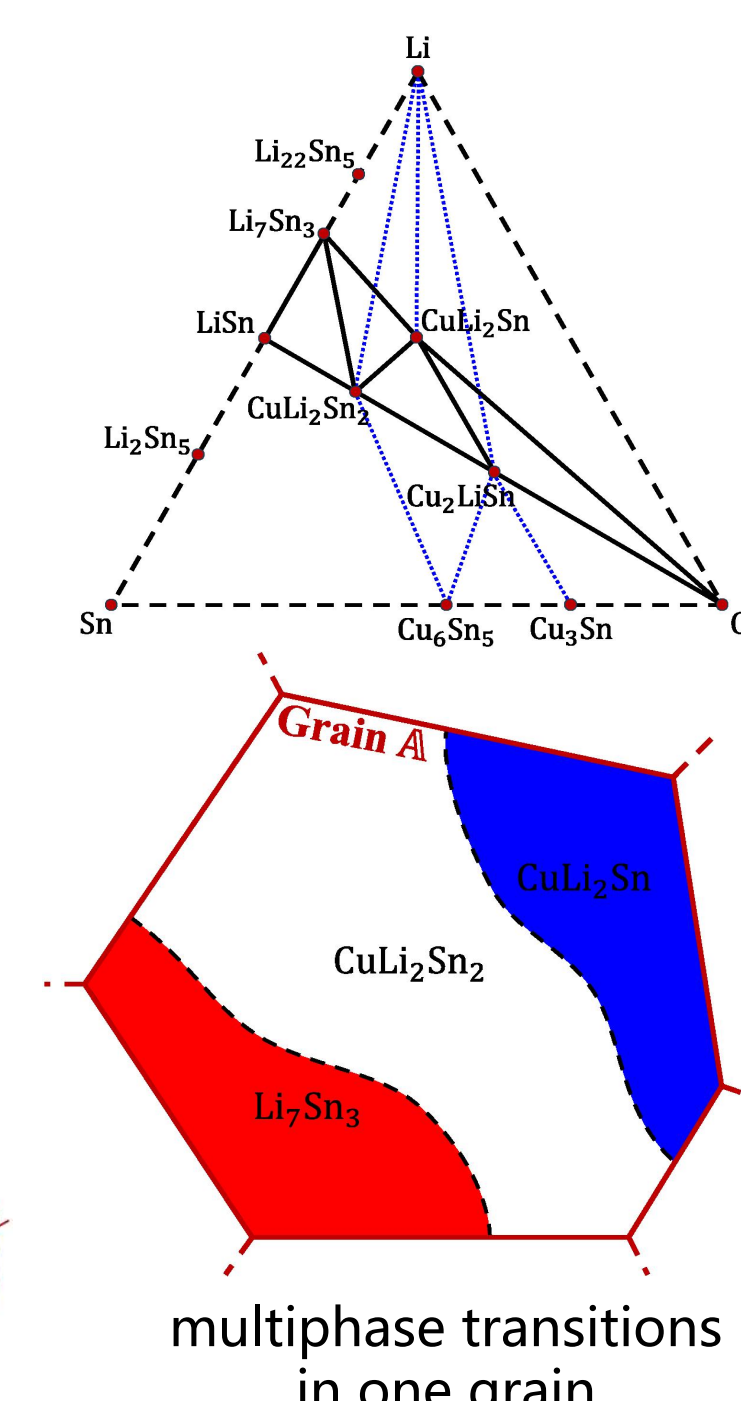
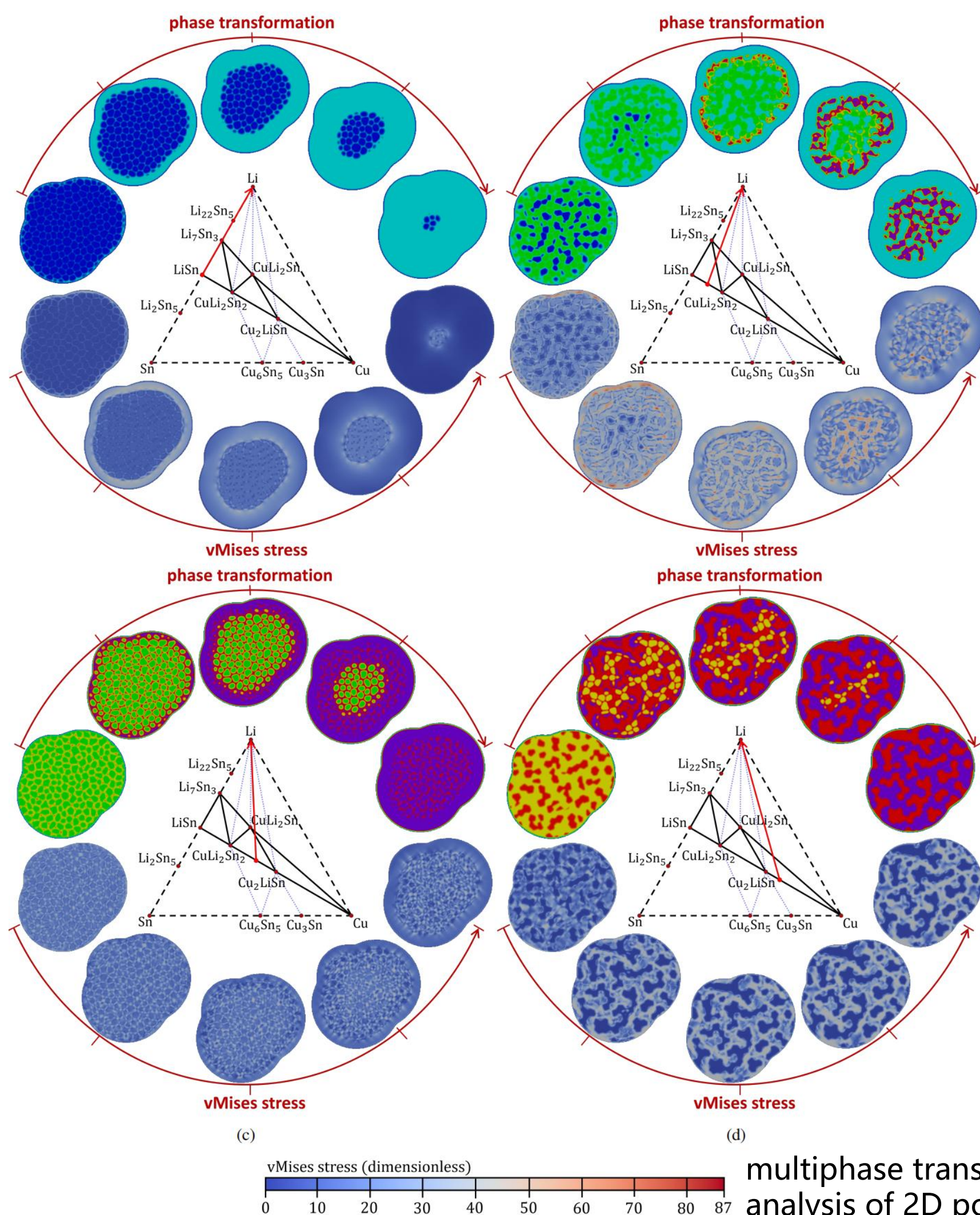
lithiation process of polycrystalline $\text{Cu}_x\text{Li}_y\text{Sn}$ nanoparticle

Methods

- multiphase-field method [1]
- smooth boundary method [4]
- grand-potential formulation
- const-current intercalation method [5]
- phase-field microelasticity theory [3]
- plastic yielding calculation [6]

Applications

- modeling of polycrystalline multiphase transitions
- modeling of 2D/3D polycrystalline nanoparticles
- lithiation of 2D/3D polycrystalline nanoparticles



reference

- [1] I. Steinbach, 17 (7) (2009) 073001.
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- [4] H.-C. Yu, et al., M. S. M. S. E. 20 (7) (2012) 075008.
- [5] S. Daubner, et al., Elec. Acta 421 (2022) 140516.
- [6] D. Schneider, et al., C. Mechanics 55(2015) 27–35.