Collaborative Research: NanoDomain Structure and Multifunctional Properties of Polymer Derived Ceramics

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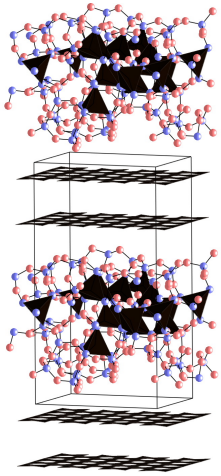
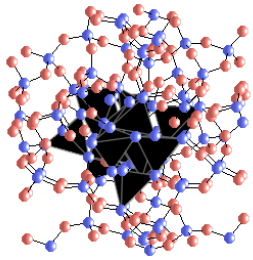
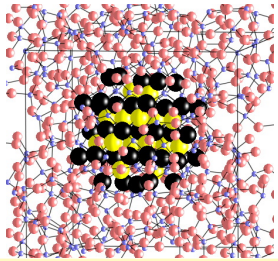
Goal: atomistic simulations to clarify microscopic structure of amorphous SiCO ceramics
Method: density functional calculations and extensive network modeling

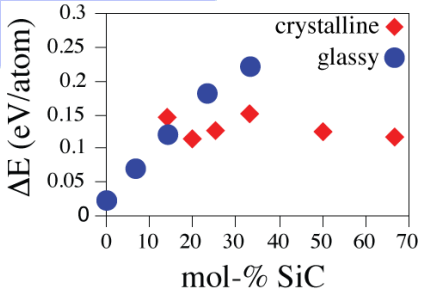


Structure & Energy

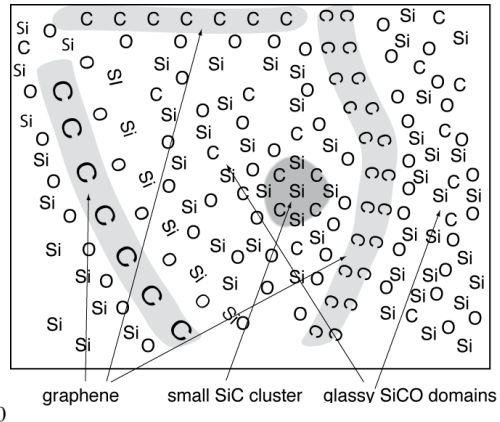
- SiC clusters precipitate in silica glass
- "C-rich" interface SiCO-C & "bonded" C-SiO_2 interface energetically not favorable
- no "stable" ternary SiCO structure

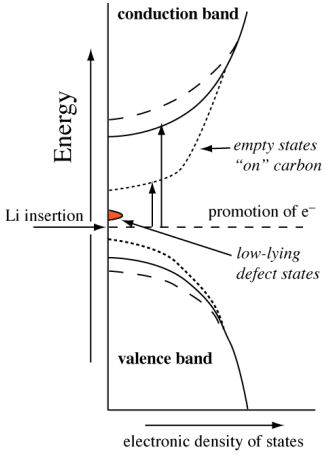






revised "Nanodomain model"





SiCO as novel Li-Anode material

- Li bonds cationic Li^+-O => e^- to unoccupied states
- "irreversible" Li attached to C-defects
- fortuitous balance between Li^+-O and electron promotion allows Li doping up to 1 Li per C !

⇒ defect-free C-rich SiCO for best anode material