Epitaxial Polymorph Stabilization through a Computational Approach to Substrate Selection

Scientific Achievement

Developed a computational framework combining calculations of formation energy, elastic strain energy and topological lattice matching to guide substrate selection for epitaxial materials growth.

Significance and Impact

This approach to substrate selection facilitates the targeted synthesis of functional materials, including metastable polymorphs and new materials.

Research Details

Pathways to synthesis: Elastic energy and topologically matching area are a first-order guide to synthesizability of a material on a substrate.

Metastable exploration: Use substrate selection as a means for stabilizing of metastable polymorphs.

VO_2 polymorph synthesis: Using the method, substrates were determined for the synthesis of VO_2 polymorphs – brookite, columbite, and anatase.

Integration into Materials Project: Soon available as part of Pymatgen and on the Materials Project website.

H. Ding *et al.*, ACS Appl. Mater. Interfaces, 2016
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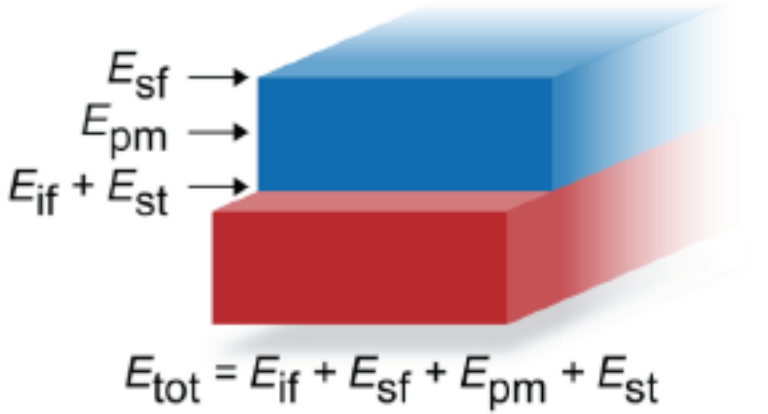

Fig. 1: Predictive model for epitaxy based on total energy

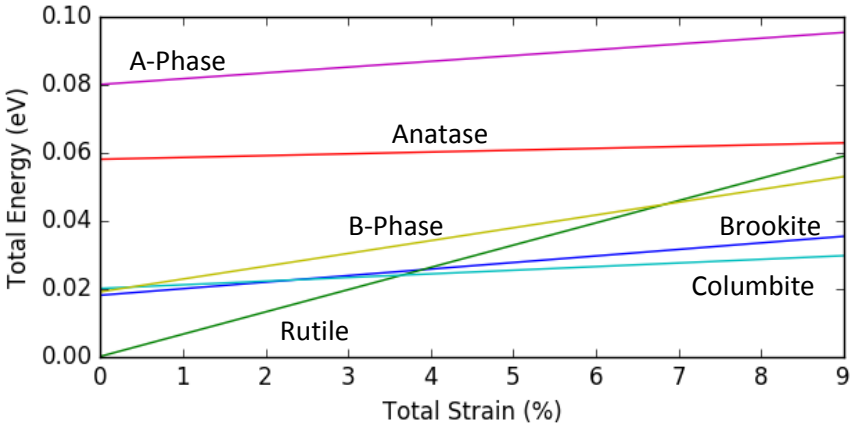

Fig. 2: Total energy of VO_2 polymorphs as a function of strain on (110)-$YAlO_3$