Mesoscale Priority Research Direction

The role of defects in phase transitions and kinetics

Opportunity

Models describing how defect accumulation leads to phase changes, shear planes, and melting are incomplete. Both the type and quantity of defects may affect phase stability, transitions, solid state reaction kinetics, and phase change kinetics. However, the mechanisms by which energy is localized at a defect and then transferred to cause a phase change are not understood.

Approach

Specifically doped materials will be compared to determine role of defect type and quantity. Phase transitions will be induced by extreme compression using diamond anvil cells and shock systems. Temperature (4000-8000K), x-ray diffraction, shear band emission, and defect emission imaging with ns resolution need to be developed to track defect and energy accumulation in a changing material.

Meso Challenge

How do nanoscale/atomistic defects affect/cause bulk property changes at the continuum level, such as melting, electron band changes, electron transport, and physical transport?

Impact

Understanding the role of defects on phase structures and transitions will lead to improved and extended phase diagrams and equations of state, and a better understanding of entropic processes. These in turn will help us to stabilize exotic and metastable phases at ambient conditions and develop new materials.

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