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Bringing together computational and experimental capabilities at the crystal scale

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Many phenomena of interest occur at the scale of crystals or are controlled be events happening at the crystalline scale. Examples include allotropic phase transformations in metals and pore collapse in energetic crystals. The research community is increasingly able to make detailed experimental observations at the crystalline scale and to inform crystal scale models using lower length scale computational tools. In situ diffraction techniques are pushing toward finer spatial and temporal resolution. Molecular and dislocation dynamics calculations are now able to directly inform mechanisms at the crystalline scale. Taken together, these factors give crystal based continuum models the ability to rationalize experimental observations, investigate competition among physical processes, and, when appropriately formulated and calibrated, predict behaviors. We will present an overview of current efforts, with some emphasis on recent work investigating phase transformations in metals and pore collapse in energetic materials. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-410456).