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High Pressure Mechanochemistry: Conceptual Multiscale Theory and Interpretation of Experiments

Valery I. Levitas

Department of Mechanical Engineering, Texas Tech University, Lubbock, USA

A simple multiscale (nano-, micro- and macro-) continuum thermodynamic theory for strain-induced phase transitions (PT) and chemical reactions (CR), as well as closed form solutions were developed which explain a number of mechanochemical phenomena. Specifically, the theory explains why the superposition of plastic shear and high pressure in rotational diamond anvil cell leads to: (a) a significant (by a factor of 3-5) reduction of PT and CR pressure and pressure hysteresis, (b) the appearance of new phases, which were not obtained without additional shear, (c) the substitution of a reversible PT by an irreversible PT, and (d) strain-controlled kinetics, (e) nanostructured phases, and (f) pressure self-multiplication effect. Additionally, the results enabled the development of new methods for control of PT and CR under plastic deformation, some of which have experimental confirmations. The results also predict the unique potential of plastic straining to produce high-strength nanostructured phases.

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