Mesoscale Priority Research Direction

Driving Structural Phase Transitions in Periodic Mesostructures

Opportunity

Driving structural phase transitions while maintaining desirable mesoscopic characteristics (e.g. periodic porosity) would permit us to greatly extend the range of physical properties that could be obtained in engineered nanomaterials. These properties could include at least optical, electronic, chemical, and mechanical. A relevant example is the amorphous carbon to diamond transition in which the properties of the transformed material are profoundly different from the starting material.

Meso Challenge

Is it possible to maintain the structure of engineered mesostructures on all length scales longer than the interatomic while simultaneously effecting a radical reorganization of the atomic configuration? For the HPHT method this involves at least fully supporting the precursor during the transition so that long range structure is preserved. *How best to match phase-transformed material and mesostructure to desired performance?* Will likely require closely integrated theoretical modeling and experimental design.

Approach

The application of high pressure and temperature (HPHT) to appropriate precursors is a promising method for driving phase transitions in engineered materials[1,2]. This approach complements well-developed routes to precursor synthesis (e.g. of periodic porous, amorphous carbon[3]). It should also be possible to selectively dope the precursor in order to produce additional desirable properties in the transformed material (consider the $(NV)^-$ defect center in diamond after the transition from an amorphous carbon which contained N impurities[2]). Approach should be generally applicable to other materials that undergo pressure-driven transitions.

Impact

Ordered mesostructured materials with novel atomic arrangements suggest a host of potential applications due to the profound changes in underlying physical properties. We may envisage for example new forms of photonic crystal with controllable pore size and optical bandgap; these structures would benefit from the transformed characteristics of the synthesized material (e.g. diamond, or a range of other phase-transformed materials) and may have advanced optical or energy applications.

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J. Crowhurst (crowhurst1@llnl.gov)
P. Pauzauskie (peterpz@uw.edu)

[1]L. Zhang, et al, PNAS, 107, 13593 (2010).
[2]P. J. Pauzauskie, et al, PNAS, 108, 8550 (2011).
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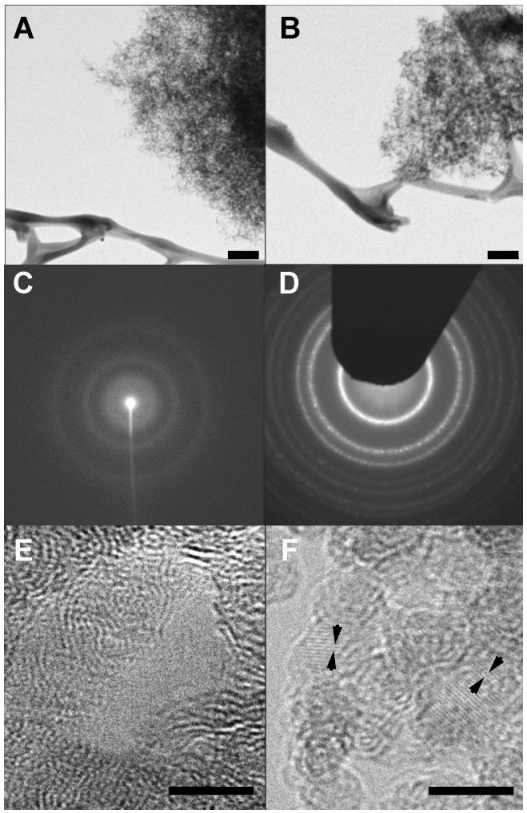

Amorphous carbon aerogel (A, C, E) and recovered nanocrystalline diamond aerogel (B, D, F) after exposure of precursor to high pressure and temperature. Scale bars in A and B: 200 nm, and in E and F: 5 nm (See Pauzauskie et al[2]).

Right: examples of periodic mesoporous carbon precursors that could be converted to diamond using the HPHT method (as was applied to carbon aerogel of random initial structure[2]). Approach should be applicable to precursors with a wide range of pore size and configuration, as well as to other materials, distinct from carbon, that also undergo pressure-driven phase transitions.