Mining for Crystals

Predicting the crystal structure of an alloy is challenging, because even small changes in composition can lead to large changes in the way the atoms prefer to coordinate. Fischer et al. have developed a technique that mines the existing crystal database to determine top candidate structures, which are then evaluated using quantum mechanical calculations. The model determines correlations for structural motifs that jointly appear in a single alloy system at different compositions, and thereby assigns probabilities to candidate structures, given those already known in the system. In one test, the authors considered the Ag-Mg alloy with 75% Mg content, for which the exact crystal structure is undetermined. The top candidate highlighted by their model was the Cu$_{2.82}$P structure, an uncommon motif that nonetheless was computed to have the lowest ground-state energy.

They also tested the model by selectively removing specific compositions from the database to see if the remaining data could be successfully used to predict the correct structures; this approach succeeded 90% of the time in placing the true missing structure among the top five candidates. — MSL

Nanoliter boxes.

Microscale Origami

Recent advances in lithography and other surface-patterning techniques have fostered construction of a wide range of microfluidic devices that offer precise control over chemical and biochemical reactions and separations at or below microliter volume scales. However, one limitation of this fabrication technology is its inherent restriction to two-dimensional device geometries.

Leong et al. overcome this limitation by patterning flat wafers with solder deposited along hinge lines. When heat is applied to melt the solder, the wafers fold spontaneously along the hinges to form cubic or pyramidal boxes, with volumes ranging from ~0.2 to 8 nl. The authors use photolithography to imprint distinct pore arrangements into the surfaces set to become the box faces. As a result, they can inject chemical reagents embedded in polymeric gels and control the rate and orientation of their release. The fabrication process is high-yielding, and when nickel is used as the substrate, the corresponding box can be manipulated with an external magnet to release its chemical cargo in a spatially selective manner. — JSY

Hematopoietic stem cells (HSCs) reside in bone marrow in a nondividing state from which they can be roused to enter the cell cycle. Noting the similarity of HSC dormancy to mammalian hibernation and Caenorhabditis elegans dauer formation, Yamazaki et al. looked at the PI3K (phosphatidylinositol 3-kinase)–Akt–FOXO signaling pathway. In quiescent cells freshly isolated from mouse bone marrow, no phosphorylated (activated) Akt was apparent and its downstream target FOXO3a was found in the nucleus; in contrast, phosphorylated Akt and FOXO3a were found in the cytoplasm of cycling progenitor cells. Cytokine treatment of quiescent cells led to polarization of the lipid raft marker GM1 ganglioside as well as phosphorylation of Akt and relocation of FOXO3a to the cytoplasm. Depleting cholesterol with β-cyclodextrin (MJCD) in order to inhibit lipid raft clustering suppressed Akt activation and FOXO3a relocation. When single HSCs that had survived without dividing for several days in the presence of MJCD, stem cell factor, and thrombopoietin were placed in MJCD-free medium, they proliferated and differentiated along various myeloid lineages in vitro and could repopulate the hematopoietic system of lethally irradiated mice. Thus, lipid raft clustering may mediate HSC emergence from dormancy via signaling pathways resembling those involved in the dauer stage. — EMA