INTERDISCIPLINARY COLLOQUIUM ON ADVANCED MATERIALS SIMULATION
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Unique properties of ferroelastic system having nanodomain structures

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We propose to alter transformation pathway and domain structure in ferroelastic systems through defect engineering to obtain special properties. The basic idea is to use local lattice distortion created by point or extended defects to prevent long-range ordered polytwin domain structures and "freeze" the ferroelastic system into a microstructural state of randomly distributed nanodomains of individual martensitic variants. By assuming that anti-site defects alter the thermodynamic stability of austenite and create local lattice distortions, we show by computer simulations using the phase field method that such a transformation pathway is possible and the unique microstructural state generated does have a rich variety of special properties, including superelasticity of nearly zero hysteresis, nearly zero thermal expansion coefficient (Invar anomaly), and low and nearly temperature-independent elastic modulus (Elinvar anomaly) over a wide temperature range. We then confirm experimentally that extra impurity doping of a conventional shape memory alloy does convert the normal long-range ordered poly-twin domain structure into a nanodomain structure of individual martensitic variants, change the large hysteresis into a slim one and widen significantly the temperature range of superelasticity. Finally we demonstrate that the same idea works for the other two ferroic systems (i.e., ferroelectric and ferromagnetic) as well.