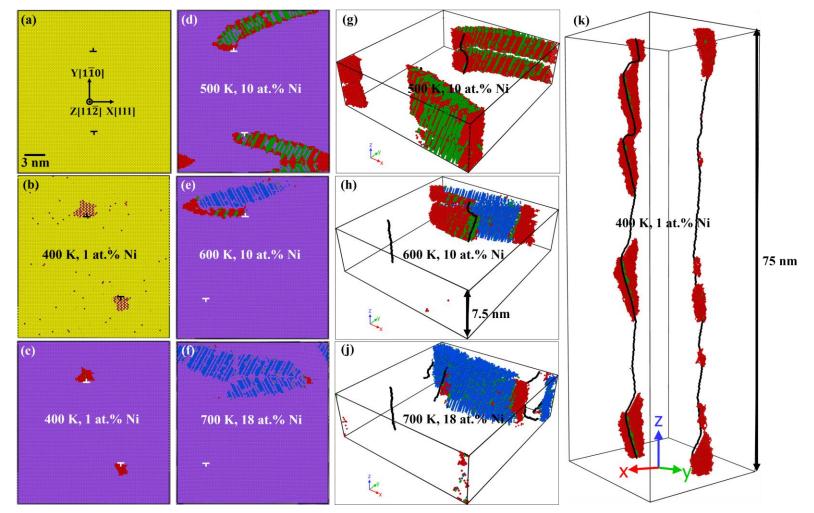


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Atomistic simulations of metals and alloys

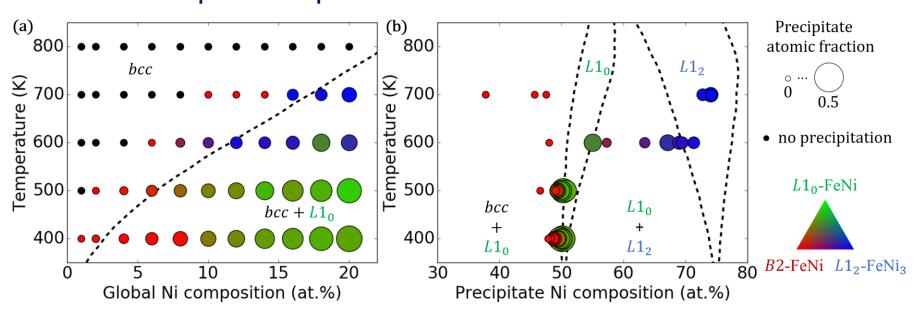




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Exploring complexion (phase) diagrams is challenging: each point requires 1 node - 64 cores - 1 week



Using optimized parallelization and machine learning techniques, we hope to build complexion diagrams based on material's properties and limited number of simulations