Martensitic phase transformations (PTs), amorphization, twinning, and dislocation motion are the main deformation mechanisms in many crystalline materials. However, the interaction between these material behaviors are not well understood. In this work, we try to understand the interaction between dislocation motion and PTs through multiscale modelling using density functional theory (DFT), in collaboration with Drs. Zarkevich and Johnson from Ames Laboratory, molecular dynamics (MD), and concurrent atomistic continuum (CAC) method. The following topics are discussed.

1. A continuum/atomistic approach for predicting lattice instability during martensitic PTs is developed for the general loading with an arbitrary stress tensor and large strains. It was applied to the transformation between semiconducting Si I and metallic Si II phases. The instability criterion represents the critical value of the modified transformation work, which is linear in normal to cubic faces components of the true stress tensor and is independent of shear stresses.

2. Starting with thermodynamic predictions and combining with MD simulations, special triaxial compression-tension states were found at which the stresses for the instability of the crystal lattice of silicon are the same for direct and reverse Si I <-> Si II PTs. This leads to unique homogeneous and hysteresis-free first-order PTs. Zero hysteresis and homogeneous transformations are the optimal property for various PT applications, which drastically reduce damage and energy dissipation.

3. DFT calculations were carried out. It turned out that the instability stress plane also exists in the stress space, which demonstrates the reliability of the MD results.

4. To scale up the simulation size, parallel algorithm was developed for a CAC method which has demonstrated to be able to reproduce phase transformation in Si. Using spatial decomposition method, the parallel efficiency reached 90% with the maximum number of processors that can be accessed, i.e., 768 from Condo at ISU. The parallel efficiency as well as the applicability of CAC in predicting dislocation-mediated plasticity in submicron-sized specimen containing billions of atoms are demonstrated.

5. At last, MD simulations showed that the martensitic PT nucleate from the dislocation site. Under hydrostatic loading, the instability pressure drops from 80GPa to 45GPa with one dislocation included. However, reduction in PT pressure saturates with increasing number of dislocations. Under uniaxial loading, the effect of dislocations is small. However, the transformation process changes to amorphization. Under shear, the dislocation pile-up against different grain boundaries in Si induces amorphous shear band. The shear stress needed for amorphization decreases almost linearly with the number of dislocations in a pile-up.