An integrated package of programs has been developed for IBM-Compatible PCs to investigate the structures and representations of crystallographic space groups. The package is implemented as a Microsoft Windows application using Borland Delphi with user code in Object-Pascal. Parts of this software have been adapted to assist in the symmetry analysis of domain structures. For a given phase transition the software identifies all domain states and finds, e.g. (i) symmetry groups of all domain states, (ii) all operations that transform a given domain state into another domain state, (iii) twinning groups and symmetries of ordered and unordered domain pairs, (iv) classes of crystallographically equivalent domain pairs with similar domain distinction. As an example of the use of the software we consider the symmetry analysis of domain structures in the 2H polytype TaSe2 in which the disordered phase has P6(3)/mmc (#194) symmetry and the ordered commensurate phase exhibits Cmcm (#63) symmetry.

We consider a model in the context of shape memory materials in which hierarchical twinning near the habit plane (austenite-martensite interface) is a new and crucial ingredient. The model includes (1) a triple-well potential in local shear strain, (2) strain gradient terms up to second order in strain and fourth order in gradient, and (3) all symmetry allowed compositional fluctuation and detailed nature of the hydrogen rearrangements responsible for the dynamic behavior. In general, these dynamics are associated with correlated hydrogen intrabond transfers responsible for creation, effective diffusion, and annihilation of WAO4 and W3A04 groups. Such groups are much more numerous in the PE than in the AFE or PE phases, so one can expect much faster dynamics in the PE phase than in the ordered phases in the coexistence regime.

A review will be presented of first-principles theoretical predictions of structural instabilities in ionically bonded solids in which one component is a molecular ion. This approach employs modified electron gas density-functional theory, together with a quantum chemical treatment of the molecular ions by the Gaussian computer code and tabulated free ion wave functions for the monatomic constituents, in order to generate parameter-free interionic potentials. These are then employed in molecular dynamics simulations which reproduce the observed structural phase transitions in a wide variety of moderately complex systems.