

MS11.05a.02 MS-WINDOWS SOFTWARE FOR SPACE GROUPS: APPLICATION TO DOMAIN STRUCTURE SYMMETRY ANALYSIS B.L. Davies, School of Mathematics, University of Wales, Bangor, Gwynedd, LL57 1UT, U.K., R. Dirl, Institut für Theoretische Physik, TU Wien, A-1040 Wien, Wiedner Hauptstrasse 8 - 10, Austria, V. Janovec, Technical University of Liberec, Halkova 6, 461 17 Liberec 1, Czech Republic, Z. Zikmund, Institute of Physics, Academy of Sciences, Na Slovance 2, 180 40 Prague 8, Czech Republic

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.

MS11.05a.03 HIERARCHICAL MICROSTRUCTURE IN STRUCTURAL PHASE TRANSITIONS. A. Saxena, S. R. Shenoy*, A. R. Bishop, Y. Wu†, T. Lookman‡, Theoretical Division, Los Alamos National Lab., Los Alamos, NM 87545, USA, *School of Physics, University of Hyderabad, Hyderabad, 500134, India, International Center for Theoretical Physics, P.O. Box 586, Trieste 34100, Italy, †Department of Applied Mathematics, University of Western Ontario, London, Ontario, N6A 5B7 Canada

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-induced strain gradient terms. The last term favors branching of domain walls which enables communication between macroscopic and microscopic regions essential for shape memory. Below the transition temperature (T_0) we obtain the conditions under which branching of twins is energetically favorable. Above T_0 a hierarchy of branched domain walls also stabilizes tweed formation (criss-cross patterns of twins). External stress or pressure modulates ("patterns") the spacing of domain walls. Therefore the "pattern" is encoded in the modulated hierarchical variation of the depth and width of the twins. We attempt to explain the four processes of the complete shape memory cycle—write, record, erase and recall—within this model. Preliminary results based on 2D molecular dynamics are shown for twins, tweed and hierarchy formation.

MS11.05a.04 PHASE COEXISTENCE IN PROTON GLASS. V.H. Schmidt, Physics Dept., Montana St. U., Bozeman, MT 59717, Z. Trybula, Inst. Molec. Physics, Polish Acad. Sci., Poznan, Poland, N.J. Pinto, Dept. Physics & Elec., U. Puerto Rico, Humacao, PR 00661, S.M. Shapiro, Physics Dept., Brookhaven Nat. Lab., Upton, NY 11973

Proton glasses are crystals of composition $M_{1-x}(NW_4)_xW_2AO_4$, where $M=K,Rb$, $W=H,D$, $A=P,As$. For $x=0$ there is a ferroelectric (FE) transition, while for $x=1$ there is an antiferroelectric (AFE) transition. In both cases, the transition is from a paraelectric (PE) state of tetragonal structure with dynamically disordered hydrogen bonds to an ordered state of orthorhombic structure. For an intermediate x range there is no transition, but the hydrogen rearrangements slow down, develop a spread in time constants, and eventually display nonergodic behavior characteristic of glasses. For x near 0, we have shown that the FE and PE phases coexist over a wide temperature range, and that similar AFE/PE coexistence occurs for x near 1. One evidence for coexistence is dielectric permittivity ϵ that decreases gradually rather than abruptly below the FE or AFE transition. Another is spontaneous polarization P_S that increases gradually rather than abruptly below the FE transition. The FE order parameters deduced from the ϵ and P_S measurements agree very well. Evidence for coexistence appears also in deuteron NMR spectra. A fourth evidence is coexistence of neutron diffraction spots for the FE and PE phases, and for the AFE and PE phases, over wide temperature ranges. Remaining to be determined are the correlation lengths for the coexisting phases, the temporal vs. spatial nature of the coexistence, and the rate 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 WAO_4 and W_3AO_4 groups. Such groups are much more numerous in the PE than in the FE or AFE phases, so one can expect much faster dynamics in the PE phase than in the ordered phases in the coexistence regime.

MS11.05a.05 STRUCTURAL PHASE TRANSITIONS IN IONIC MOLECULAR SOLIDS*. John R. Hardy, Department of Physics & Astronomy, 260 Behlen Lab University of Nebraska-Lincoln Lincoln, NE 68588-0111

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.

Specific examples to be discussed will include incommensurate behavior in the A_2BX_4 compound K_2SeO_4 and its isomorphs, and order-disorder transitions in KNO_3 and $NaNO_2$. These findings will be used to illustrate the degree to which transitions in these and other similar solids are governed by ionic size, geometry, and overall symmetry considerations relating to the packing of molecular groups into spatially periodic arrays.

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