21-Crystallography at Non-Ambient Temperatures and/or Pressures; Phase Transitions

MS-21.03.06

MICROSTRUCTURAL DEVELOPMENT RELATED TO PHONON ANOMALIES LEADING TO DISPLACIVE TRANSFORMATIONS IN METALLIC PHASES.

By L.E. Tanner, A.J. Schwartz*, D. Schryvers[1] and S.M. Shapiro[2], Department of Chemistry and Materials Science, Lawrence Livermore National Laboratory, Livermore, CA, U.S.A. [1] Electron Microscopy for Materials Research, University of Antwerp (RUCA), Antwerp, Belgium, [2] Physics Department, Brookhaven National Laboratory, Upton, NY, U.S.A.

The phonons of crystalline phases (pure metal and alloyed) that undergo first-order displacive transformations on cooling exhibit anomalously low energies along those branch(es) related to the atomic displacements of the ensuing structural changes. Present at elevated temperature equilibrium, these effects become more pronounced as $T \rightarrow T_c$ (or M_s), the bulk transformation temperature, though the "softening" is never complete at T_c. The coupling between the soft phonons and local parent lattice distortions (defects) sets the stage for heterogeneous nucleation. [Phys. Rev. B **44**, 9301 (1991); Ultramicroscopy, **37**, 241 (1990)]. HRTEM and neutron scattering observations of Ni-Al, Ti-Ni-Fe, Ti-Pd-Fe, Ti-Pd-Cr, Ti-Mo and Zr-Nb transformations illustrate the foregoing and will be discussed in terms of nonclassical heterogeneous nucleation theory.

This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

MS-21.03.07

DOMAIN WALLS IN CRYSTALS WITH INCOMMENSURATE PHASES.

By Y. Ishibashi, Synthetic Crystal Research Laboratory, School of Engineering, Nagoya University, Nagoya 464-01, Japan.

The domain wall is a transient region where two domains with different values of the order parameter meet. Fundamental features of domain walls, like the spatial variation of the order parameters in the wall, the wall energies and the activation energies, are discussed on the basis of the Landau-type thermodynamic potentials applicable to crystals, which have the incommensurate phases. The domain walls to be considered will be those between two commensurate domains, two incommensurate domains, and a commensurate domain and an incommensurate domain. It will be clarified how the factors stabilizing the incommensurate phase should affect characteristics of the domain walls. In particular, the contribution from the Lifshitz invariant to the wall structure and so on will be discussed.

MS-21.03.08

PHASE TRANSITIONS IN QUASICRYSTALS

By F. Dénoyer*, P. Launois and M. Lambert, Laboratoire de Physique des Solides, Associé au C.N.R.S., Batiment 510, Université Paris-Sud, 91405 Orsay Cédex, France.

The Al-Cu-Fe equilibrium diagram has been the subject of many experimental investigations. It has been shown that a phase transformation between a high temperature icosahedral quasicrystalline phase and a low temperature rhombohedral microcrystalline phase occurs in the vicinity of the composition 63.5-24-12.5. The material also exhibits an "intermediate" modulated quasicrystalline state.

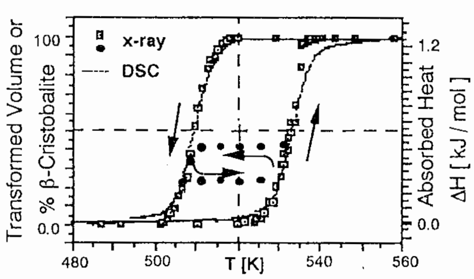
In this short lecture, we will perform a review of the experimental and theoretical works related to these phase transformations.

MS-21.03.09

ATHERMAL TRANSFORMATION KINETICS AND THERMAL HYSTERESIS AT WEAKLY FIRST ORDER PHASE TRANSITIONS.

By W.W. Schmahl , Fachbereich Materialwissenschaft, Technische Hochschule Darmstadt, Germany

Although thermal hysteresis is a common feature of first order phase transitions, there is only rudimentary knowledge about its origin and characteristics. The non-quenchable α/β-cristobalite phase transition near 520 K is associated with a 'thermal' hysteresis of ± 15 K and α/β-phase coexistence in the hysteresis loop. Measurements by x-ray diffraction (0.03 K/min) or DSC (5K/min) give practically the same result (see figure). The transformation proceeds instantly as a function of temperature; thermal activation is not a relevant factor. These 'athermal' features are similar to martensitic transformations in metals and alloys and to field-reversal hysteresis in ferroics. The bulk Landau-free energy isotherms suggest that local strain-fields control nucleation and initiate both phase coexistence and 'thermal' hysteresis.



MS-21.03.10

A 2Θ- RESOLVED HADOX STUDY OF $BaTiO_3$ LINZ CRYSTALS.

By H. Onitsuka, M. Hatakeyama, Y. Soejima and A. Okazaki*, Department of Physics, Kyushu University, Fukuoka 812, Japan.

X-ray diffraction intensities in a reciprocal-lattice plane can be measured with high resolution in two dimensions by improved high-angle double-crystal X-ray diffractometry (HADOX). In addition to the original experimental arrangement in HADOX, two slits have been introduced: one for limiting the area of the specimen crystal to be examined, and the other for defining the resolution of 2θ. Thus we can correlate the original ω scanning of the specimen with the 2θ scanning of the detector, and determine two-dimensional intensity distribution. This technique, named the 2θ-resolved HADOX, enables us to determine separately and precisely changes in lattice constants and changes in crystal orientation. This is required in the structural study of first-order transitions. The method has been applied to the cubic-to-tetragonal phase transition in $BaTiO_3$ Linz crystals grown by the method of top-seeded solution growth; the results are compared with those of previous experiments on butterfly crystals of $BaTiO_3$. It is found that the two types of crystals behave in quantitatively different manners around the transition: the transition temperature, the temperature range of two-phase coexistence etc. are different. In

