M07.0C Phase Transitions

Chair: J.M. Pérez-Mato
Co-Chair: U. Bismayer

Attendance: 200

The well-attended Phase Transitions Micro-symposium opened with an excellent review of the application of theoretical methods like the combination of quantum mechanical Density Functional Theory (including the WIEN code) with statistical thermodynamics to the study of phase transitions such as the fcc-bcc Bain transformation (K. Schwartz, Austria). This was followed by a lively discussion of the crystal chemistry underlying the inherent displacive flexibility and associated susceptibility to phase transformation of framework structures and compositionally flexible solid solutions (R.Withers, Australia). The characteristic domain textures associated with ferroelastic phase transformations (needles, trumpets, wiggled walls), the nano-structure of twin boundaries and the effect this has upon physical properties such as ion transport along twin walls (E.Salje, UK) were the subject of the next presentation. O.Hernandez (France) discussed recent results on modulated phases of BCCD and the anharmonicity of the associated atomic modulation functions. An apparent conflict betweenneutron and X-ray structure refinements as to the degree of anharmonicity in BCCD was shown to be due to the fact that X-rays induce an unusual time decay of the intensity of high order satellite peaks. The session was concluded by R.Angel (Germany) who presented new results of a detailed investigation of a high pressure incommensurate to normal structural phase transition which takes place at ~1.7GPa in akermanite.

Ray Withers/Ulrich Bismayer