

**PS11.10.10 MONTE CARLO STUDY OF THE BEHAVIOUR OF THE LANDAU FREE ENERGY AND ORDER PARAMETER IN THE 3D- $\alpha^4$  MODEL.** S. Radescu\*, I. Etxebarria\*\* and J.M. Perez-Mato\*\*, \*Departamento de Fisica Fundamental y Experimental, Universidad de La Laguna, La Laguna E-38205, Tenerife, Spain, \*\*Departamento de Fisica de la Materia Condensada, Facultad de Ciencias, Universidad del Pais Vasco, Apdo 644, E-48080 Bilbao, Spain

We have investigated the features of the structural second order phase transitions modelled by a simple three dimensional  $\alpha^4$  model within the framework of the phenomenological Landau theory. At each fixed temperature we have computed the distribution of the order parameter via the Monte Carlo method using a Metropolis statistical sample scheme with a  $10 \times 10 \times 10$  grid, and from this histogram distribution we have obtained the value of the primary order parameter,  $\langle Q \rangle$ , as a function of temperature. We have studied the behaviour of the Landau coefficients and of the order parameter as a function of the temperature, and have obtained the critical temperature for the transition. We have also compared the results of our study with the analytical results for the cases of high and low temperature (displacive and order-disorder limits, respectively). Considering different model parameters ranging from the typical displacive analytical limit to a nearly pure order-disorder limit and taking into account the results of a simulation for the 3D Ising model at zero magnetic field we observe a simple law which can be related to the displacive degree of the system. In particular, we find the important result that for a large interval of temperatures "outside" any possibly critical region a simple non-classical  $(T_c - T)^\alpha$  power law accurately models the temperature dependence of the order parameter. The value of the exponent  $\alpha$  has been proposed to be related to the displacive/order-disorder degree of the system.

References:

- G.Ciccotti, D.Frenkel and I.R.MacDonald Simulation of liquids and solids: Molecular Dynamics and Monte Carlo methods in statistical mechanics (North Holland, Amsterdam, 1990)  
A.D.Bruce Monte Carlo Methods in Statistical Physics (Springer, 1979)

**PS11.10.11 THE USE OF ZONE CONTROL CHARTS IN QUANTITATIVE XRAY POWDER PHASE ANALYSIS TO INSURE QUALITY CONTROL.** Jeffery N. Dann and Harry O. Fassett, Osram Sylvania Inc. Tonawanda PA 188480504

Statistical Process Control (SPC) charts, or Shewhart Charts are used to monitor reference or control samples, to insure that the calculated phase analyses of unknown samples are not in error due to equipment or sample preparation variability.

As long as the calculated amounts of phases present in the control samples do not vary from the historic mean values by more than three standard deviations, the calculated amounts of phases in unknown samples are assumed to be correct.

Zone Control Charts make the plotting of data points less difficult for X-ray Diffraction operators than the standard control charts. Examples will include determination of  $Ba_5Si_8O_{21}$  in  $BaSi_2O_5$ ,  $Sb_4O_5Cl_2$  in  $Sb_2O_3$ , and  $Y_3TaO_7$  in  $YTao_4$ .