05.1.01 TRANSITIONS BETWEEN PHASES WHICH HAVE NO GROUP-SUBGROUP RELATIONSHIP. By P. Delapalme, Groupe de Physique Théorique, UER de Sciences, 33 rue Saint-Leu, 60019 Amiens Cedex, France.

In several substances, among which figures a large fraction of the elements, there are transitions which are not group-subgroup related. For these substances the question is stated whether some general properties can be derived from the corresponding structural changes or if their phenomenological features are unpredictable. We examine the various situations which may be encountered on that score. Two main classes of transitions are distinguished, owing to an essential difference in their microscopic mechanism: 1) A first class contains the transitions for which the rearrangement of structure is such that no rupture of the atomic bonds occurs, but only displacements of atoms from one equilibrium site to another. In this case it is shown that the space groups $G_1$ and $G_2$ of the two phases possess either a common parent group or a common subgroup. In both cases a phenomenological description can be performed providing one or several order-parameters. A number of illustrative examples are discussed among which, among others, tetraboride, lithium iodide and the $M_2'W_{17}^\text{II}(XO_5)$ family (B. Jolibois et al., Acta cryst. (1980) B36, 2577).

2) A second class contains substances for which the structure of one phase is broken down and reconstructed in a new one forming a modified packing of the atoms with a partial rupture of the atomic bonds. In this case it is shown that two sorts of parameters have to be used for a phenomenological description. A first set, composed by order-parameters of the Landau-type describes the phase-change associated to the preserved portion of the system. An additional set of parameters expresses the loss of informations corresponding to the restructuring part of the lattice and indicates the disruptions undergone by the system. Examples of such parameters are given for experimentally observed martensitic transformations and for transitions taking place within the elements.

05.1.02 A VARIATIONAL APPROACH TO SHORT-RANGE ORDER INTENSITY. By J. M. Sanchez and D. de Fontaine, Department of Materials Science and Mineral Engineering, University of California, Berkeley, CA 94720, USA.

A staggered field method is proposed for calculating the short-range order (SRO) intensity in binary alloys (ising systems, in general) using the functions generated by the cluster variation method (CVM) as approximately free energy expressions. The method is exact when the CVM free energy function is also exact, as in the one-dimensional Ising model, the integrated SRO intensity remains strictly constant at all temperatures. For higher-dimensional cases, the calculated integrated intensity can be used as a sensitive measure of the level of approximation, the CVM performing well at high temperature and breaking down as expected, near critical points. The calculated SRO intensity reduces to the well-known van der Waals-Clapp-Hoss formula when the free energy is written in the Breg-Williams approximation. Higher CVM approximations are seen to behave much better in terms of the constancy of integrated SRO. The new CVM-derived SRO intensity is also consistent with the CVM derivation of corresponding phase diagrams. Theoretical calculations will be compared to experimental SRO intensity data for the Cu-Au system.

05.1.03 THE USE OF GROUP THEORY FOR CALCULATING THE CONFIGURATIONAL ENTROPY IN THE CLUSTER VARIATION APPROXIMATION. By D. Gratias*, J. M. Sanchez and D. de Fontaine, Department of Materials Science & Mineral Engineering, University of California, Berkeley, CA 94720, USA. (*) Permanent address: C.E.C.M./CNRS, 15 rue G. Urbain, 94400-Vitry, FRANCE

One of the difficulties encountered in the Cluster Variation Method (CVM) is that of calculating approximate expressions for the number $\Omega$ of configurations of a crystal lattice having specified distributions of clusters (pairs, triangles, ...). The methods proposed up to now are based on the knowledge of the number of equivalent subclusters contained in a given basic cluster. A simple way of determining these numbers is proposed for any type of cluster in a general structure based on group theory considerations: given two clusters $A$ and $A'$ ($A'$ being a subcluster of $A$) and their normalizer $N_A$ and $N_{A'}$ in the symmetry group $G$ of the crystal, let $N_{A'}$ be its intersection group; then the index of $N_{A'}$ in $N_A$ represents the number of $A'$ equivalent clusters contained in $A$, while the index of $N_{A'}$ in $N_A$ represents the number of $A'$ equivalent clusters containing $A'$. The determination of these indices for all clusters involved in the chosen approximation leads directly to the entropy expression. Moreover, a general expression for $\Omega$ can be given, which leads to an iterative formula relating any two successive orders of approximation.