Materials Science and Technology Division

Materials Theory Seminar

"Solution of complex problems of phase transformations using combination of first-principles and model methods"

German Samolyuk
Ames Laboratory/Iowa State University

Thursday, August 21, 2008
10:00 a.m.
4500S, A-177

Abstract:

The description of phase equilibriums and transformations is very important and complex problem of the condensed mater physics. The general method used in this type of investigation is to reduce problem to the model, with parameters obtained from first-principles calculation, and then solve the model.

This general approach was applied to:

1. Explanation of high-temperature ferromagnetism of $GdFe_{220}$. It is shown that for such a systems rhigh T_C $GdFed_{220}$magnetic ordering can be understood in the conceptually simple of large Heisenberg moments associated with the Gd^{3+}ion S=7/, which is embedded in the Nearly Ferromagnetic Fermi Liquid (NFFL). The NFFL character of the prototype system $YF_{220}$is discussed using results of electronic structure calculation and Stoner criteria.
2. Heisenberg model approach is used to investigate unusual magneto-structural phase transition, giant magneto-caloric and magneto-resistance effects in extraordinary responsive Gd_{522}material.
3. The fundamental master equation is used to develop a consistent description of the evolution of non-equilibrium atomic distributions. The methods developed are used for detailed studies of problems of the kinetics of the $L1_0$type orderings. The "tweed" and "twin"stages of micro- structural evolution are discussed.

Host: Roger Stoller