Monte Carlo calculations of Curie temperature of $Y_{1-x}Gd_x(Fe_{1-y}Co_y)_2$ pseudobinary system

B. Wasilewski$^1$ and M. Werwiński$^1$

$^1$Institute of Molecular Physics Polish Academy of Sciences,
M. Smoluchowskiego 17, 60-179 Poznań

The $Y_{1-x}Gd_x(Fe_{1-y}Co_y)_2$ system belongs to Laves phases [1,2], which are binary close-packed structures with the chemical composition AB$_2$. Our main result is the dependence of the Curie temperature on the Gd and Co concentrations of the $Y_{1-x}Gd_x(Fe_{1-y}Co_y)_2$ system, obtained by fashioning the Heisenberg model Hamiltonian of the mentioned system with Monte Carlo simulations using parameters from the first-principles calculations. Furthermore, we investigate the dependence of exchange integrals on inter-atomic distance and study the behavior of total and partial magnetic moments as calculated from the first principles. For the $Y_{1-x}Gd_xFe_2$ system we reproduced the linear dependence of $T_C$ on Gd concentration $x$ and for the $Y(Fe_{1-y}Co_y)_2$ and Gd$(Fe_{1-y}Co_y)_2$ we reproduced the characteristic Slater-Pauling-like dependence of $T_C$ on Co concentration $y$.

References:
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