## Structural and magnetic properties of Cr telluride-selenide alloys

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We present the results of theoretical study of magnetic and structural properties of Cr telluride-selenide alloys having trigonal crystal structure. Both ground state and temperature-dependent magnetic properties of the $Cr_x(Te_\alpha Se_\beta)_2$ alloys have been investigated in a wide region of $\alpha : \beta$ ratios with various Cr content. Theoretical results are compared with the experimental ones.

The ground state properties have been studied on the basis of electronic structure calculations using the Korringa-Kohn-Rostoker (KKR) band structure method. The substoichiometry and the disorder in the chalcogenide sub-lattice has been treated by means of the Coherent Potential Approximation (CPA) alloy theory. Magnetic properties at finite temperature have been studied by means of Monte Carlo simulations on the basis of a classical Heisenberg Hamiltonian and the exchange coupling parameters calculated from first principles. This approach allowed to determine the critical temperature in good agreement with experiment.

9.7 cm

13.4 cm

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