MAGNETIC AND NONMAGNETIC DOPANTS IN Mg_2Si THERMOELECTRIC MATERIAL STUDIED WITH KKR-CPA METHOD

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Mg_2X ($X = \{Si,\ Ge,\ Sn\}$) compounds are widely considered as promising thermoelectric materials. Appropriate doping enhances thermoelectric performance and it is of prime interest to investigate the influence of impurity states on electron transport properties. Some magnetic and nonmagnetic dopants diluted in anti-fluorite structure Mg_2Si semiconductor were studied from electronic density of states and dispersion curves using the Korringa-Kohn-Rostoker method with the coherent potential approximation. The site preference of impurity was examined in view of the formation energy. The charge conductivity n- or p-type was determined from the Fermi level position at the conduction or valence band edges, respectively. Furthermore, the effect of semiconductor-metal crossover on thermopower was studied from the Fermi surfaces. The Seebeck coefficient was estimated from the Mott's formula with the use of computed velocities and lifetimes of electrons. The transition metal impurities diluted in Mg_2Si were found to exhibit a large spin-polarization of d-states, being however closer to half-metallic ferromagnetism than to diluted magnetic semiconductivity. One of us (P.Z.) acknowledges the partial support by the EU Human Capital Operation Program, Polish Project No. POKL.04.0101-00-434/08-00.

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