World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:12, No:03, 2018

Temperature Dependent Interaction Energies among X (=Ru, Rh) Impurities in Pd-Rich PdX Alloys

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Abstract : We study the temperature dependence of the interaction energies (IEs) of X (=Ru, Rh) impurities in Pd, due to the Fermi-Dirac (FD) distribution and the thermal vibration effect by the Debye-Grüneisen model. The n-body (n=2~4) IEs among X impurities in Pd, being used to calculate the internal energies in the free energies of the Pd-rich PdX alloys, are determined uniquely and successively from the lower-order to higher-order, by the full-potential Korringa-Kohn-Rostoker Green’s function method (FPKKR), combined with the generalized gradient approximation in the density functional theory. We found that the temperature dependence of IEs due to the FD distribution, being usually neglected, is very important to reproduce the X-concentration dependence of the observed solvus temperatures of the Pd-rich PdX (X=Ru, Rh) alloys.

Keywords : full-potential KKR-green’s function method, Fermi-Dirac distribution, GGA, phase diagram of Pd-rich PdX (X=Ru,Rh) alloys, thermal vibration effect
Conference Title : ICMP 2018 : International Conference on Materials and Properties
Conference Location : Singapore, Singapore
Conference Dates : March 22-23, 2018