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Finite temperatures and the alloy analogy model

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Theoretical description of nonzero temperatures, including effects of spin fluctuations, has been problematic for a long time. In recent years, the alloy analogy model (AAM) became popular for a treatment of finite-temperature effects from the first principles [1]. Phonons, described as uncorrelated displacements of atoms, can be combined with spin fluctuations (magnons) and chemical disorder. The realistic inclusion of spin fluctuations is crucial especially for spintronic properties such as the spin polarization of the electrical current. The AAM within the tight-binding linear-muffin-tin orbital method and the coherent potential approximation (CPA) successfully describes electrical transport at nonzero temperatures even in multisublattice half-Heusler alloys [2]. In the previous studies (i) the Debye theory was employed for a conversion between displacements and temperature, (ii) the total magnetization as a function of temperature was obtained from experiments, and (iii) a change of a volume with temperature was neglected. These simplification will be addressed in details. A route to overcome it by proper ab initio approaches is envisaged. Obtained corrections are a few percents (compared to the previous techniques) for some materials. However, this more precise approach is essential for systems where the Debye theory fails. Moreover, the description of finite temperatures is finally obtained completely from the first principles. It is done by synergizing precise supercell methods with the numerically efficient CPA. We will present the usage of novel techniques for pure transition metals, both nonmagnetic and magnetic, but it can be easily generalized for more complex systems, such as previously studied random and ordered [2] alloys.

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