Thermal Spin Fluctuation in Paramagnetic Fe and Stainless Steel Fe15Cr15Ni from First-Principles

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The great variety intrinsic properties of Fe and its alloys are dependent on the magnetic state of it. At thermal excitations, the atomic moment or spin fluctuation becomes an important question in itinerant-electron systems. In the present work, the spin fluctuation distribution is established using Boltzmann statistical scheme based on series constrained local magnetic moment modelings. The temperature dependence of elastic constants (c' and c_{44}) of paramagnetic (PM) bcc Fe, fcc Fe, and fcc Fe15Cr15Ni are investigated under thermo-magneto-volume coupling with the consideration of spin fluctuation. According to the theoretical predictions, in PM bcc Fe, the spin fluctuation tends to improve the decreasing rate of elastic constants when the temperature increases; and it slows down the decreasing process in fcc Fe and austenitic stainless steel Fe15Cr15Ni. With respect to pure fcc Fe, spin fluctuation has greater contributions to the elastic properties of stainless steel Fe15Cr15Ni. At 1600 K, the decreasing rate of c' and c_{44} contributed from volume expansion could be canceled out by about 40 % and 10 %, respectively, by thermal spin fluctuation in Fe15Cr15Ni.

Keywords: Spin fluctuation; paramagnetic Fe; austenitic stainless steel Fe15Cr15Ni; elastic constants; temperature

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